

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
 Data File : BF128276.D
 Acq On : 16 May 2022 19:14
 Operator : CG\JU
 Sample : N2832-08
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB10

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128276.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.116	478	481	486	rVB	34789	38291	1.86%	0.171%
2	5.316	511	515	522	rBV	60380	78633	3.83%	0.352%
3	5.510	544	548	562	rBV	2109228	1941681	94.56%	8.687%
4	6.516	714	719	722	rBV	2006371	1971587	96.01%	8.821%
5	6.887	778	782	785	rBV	570996	517698	25.21%	2.316%
6	7.298	849	852	863	rVB	22289	29653	1.44%	0.133%
7	7.451	873	878	881	rBV	1434725	1304286	63.52%	5.835%
8	8.063	979	982	993	rBV	53171	83922	4.09%	0.375%
9	8.169	996	1000	1003	rBV	751529	632238	30.79%	2.829%
10	9.016	1140	1144	1152	rBV	86226	102119	4.97%	0.457%
11	9.239	1178	1182	1186	rBV	2147653	2053468	100.00%	9.187%
12	9.351	1197	1201	1205	rVB	40442	38960	1.90%	0.174%
13	9.928	1295	1299	1302	rBV	704182	642799	31.30%	2.876%
14	10.716	1429	1433	1441	rBV	1430543	1265895	61.65%	5.664%
15	11.292	1528	1531	1539	rBV	148040	153844	7.49%	0.688%
16	11.416	1548	1552	1555	rBV	763775	628433	30.60%	2.812%
17	11.457	1555	1559	1563	rVB2	22000	27158	1.32%	0.122%
18	11.933	1636	1640	1645	rBV	90913	95241	4.64%	0.426%
19	12.498	1734	1736	1739	rVB	35728	28904	1.41%	0.129%
20	12.633	1756	1759	1762	rBV	36196	34455	1.68%	0.154%
21	12.669	1762	1765	1771	rVB	28558	27334	1.33%	0.122%
22	12.863	1792	1798	1800	rBV	47492	48205	2.35%	0.216%
23	12.886	1800	1802	1811	rVB4	19979	28034	1.37%	0.125%
24	13.004	1817	1822	1825	rVB	2135257	1886680	91.88%	8.441%
25	13.216	1854	1858	1868	rBV	105755	188017	9.16%	0.841%
26	13.439	1892	1896	1898	rVB	29867	24907	1.21%	0.111%
27	13.557	1913	1916	1919	rBV2	36177	41738	2.03%	0.187%
28	13.680	1934	1937	1940	rBV	36958	36137	1.76%	0.162%
29	13.892	1969	1973	1989	rBV	538238	1105780	53.85%	4.947%
30	14.021	1993	1995	1998	rVB	43892	42617	2.08%	0.191%
31	14.063	1998	2002	2005	rBV	677484	586732	28.57%	2.625%
32	14.151	2014	2017	2021	rBV2	30790	38283	1.86%	0.171%
33	14.204	2023	2026	2028	rVV	46440	39823	1.94%	0.178%
34	14.233	2028	2031	2039	rVB2	109642	178498	8.69%	0.799%
35	14.327	2044	2047	2051	rVB	53948	52213	2.54%	0.234%
36	14.533	2074	2082	2097	rBV2	789566	1780901	86.73%	7.968%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
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37	14.810	2125	2129	2133	rBV2	131619	168367	8.20%	0.753%
38	14.857	2133	2137	2151	rVV	254817	545134	26.55%	2.439%
39	14.968	2153	2156	2161	rVB	110456	115822	5.64%	0.518%
40	15.162	2184	2189	2193	rBV	586039	654934	31.89%	2.930%
41	15.210	2193	2197	2202	rBV2	238018	485977	23.67%	2.174%
42	15.557	2250	2256	2260	rBV	339429	463402	22.57%	2.073%
43	15.762	2286	2291	2301	rBV3	114485	180660	8.80%	0.808%
44	15.998	2325	2331	2337	rVB	412608	607087	29.56%	2.716%
45	16.121	2349	2352	2365	rVB	126581	220056	10.72%	0.985%
46	16.815	2465	2470	2479	rVB	80767	161087	7.84%	0.721%
47	17.315	2550	2555	2561	rVB	105632	191801	9.34%	0.858%
48	17.727	2619	2625	2633	rVB4	146190	348655	16.98%	1.560%
49	18.015	2669	2674	2693	rVB4	93144	433057	21.09%	1.938%

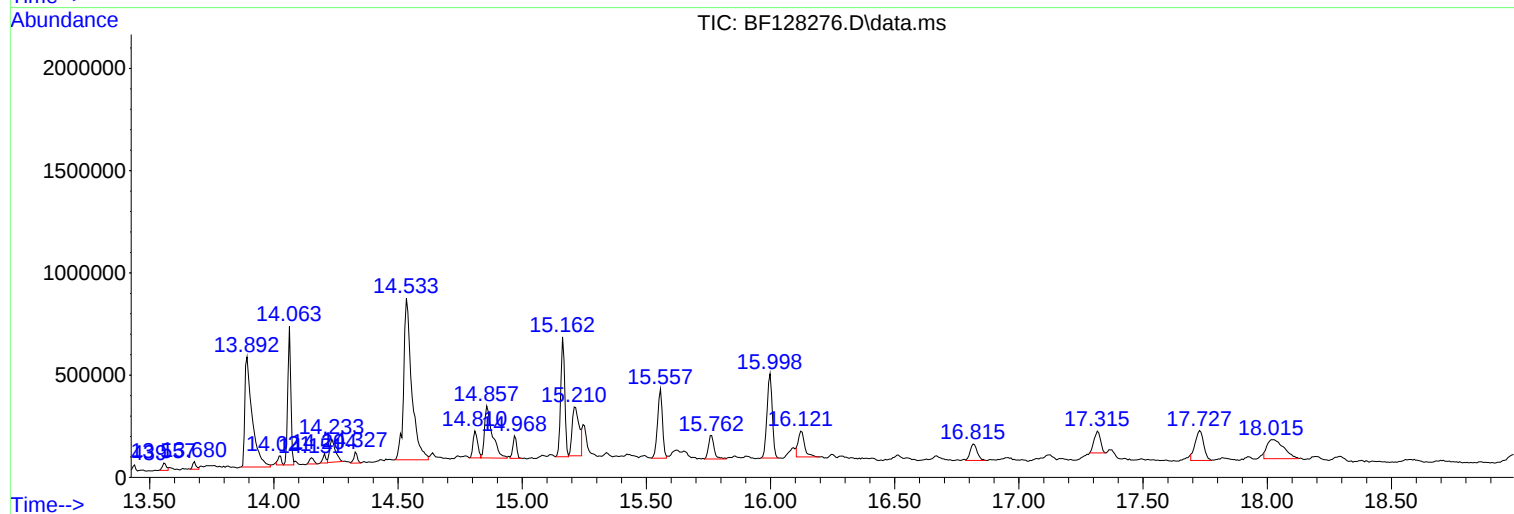
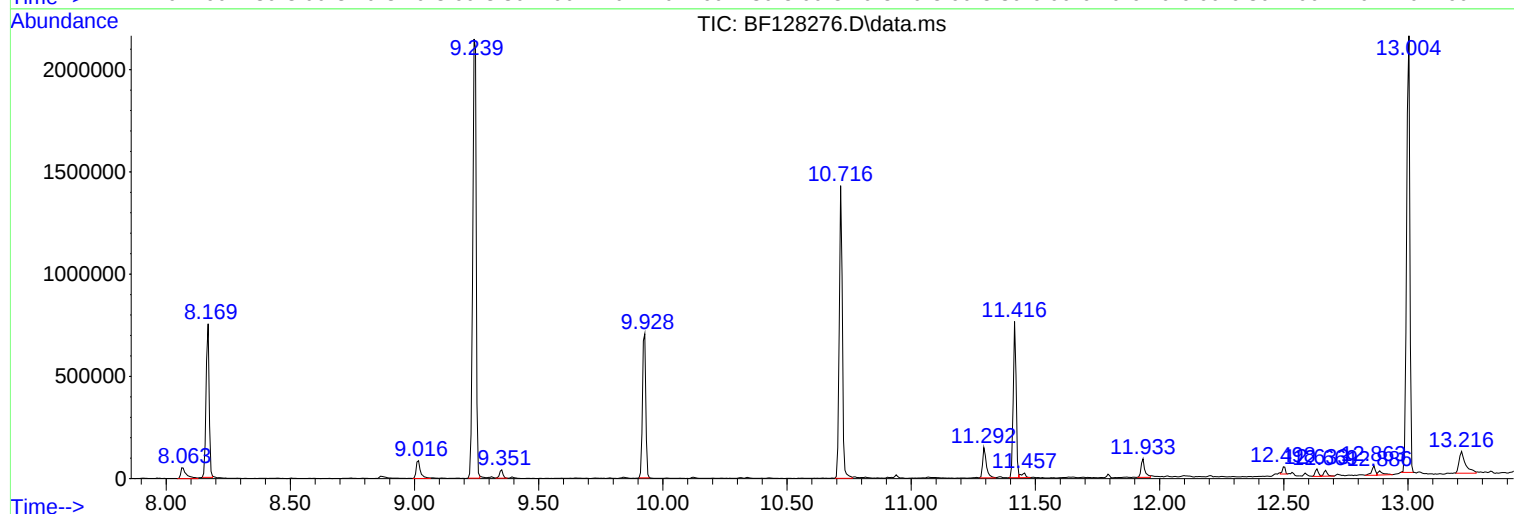
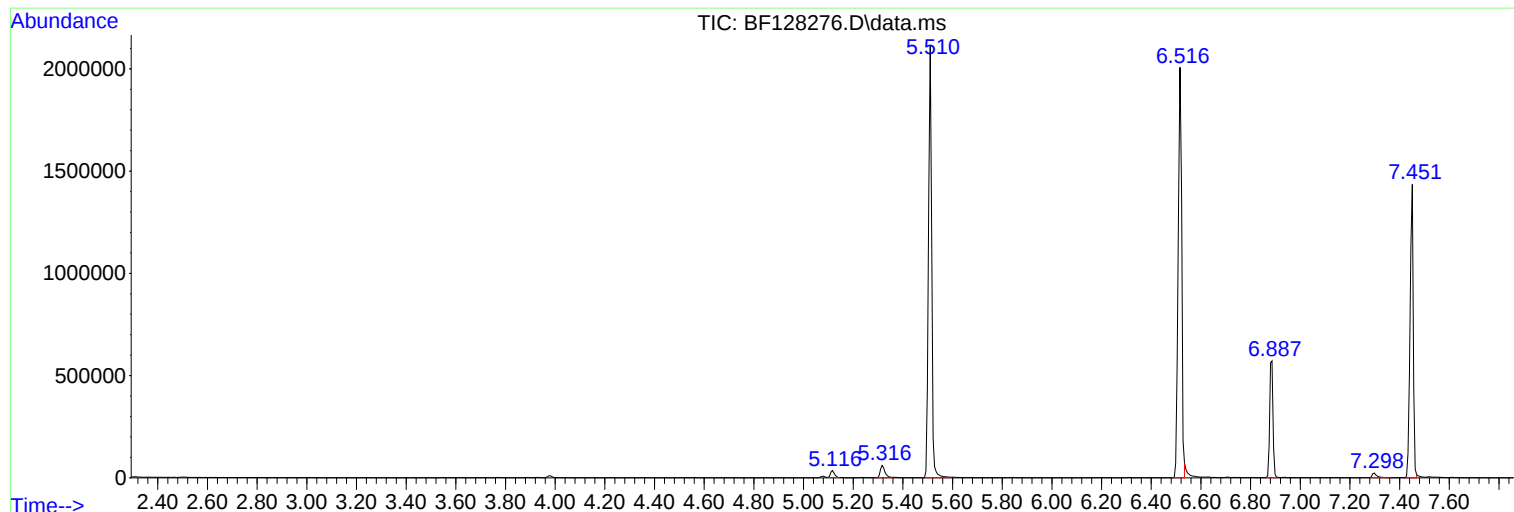
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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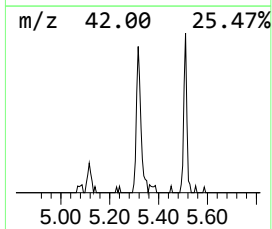
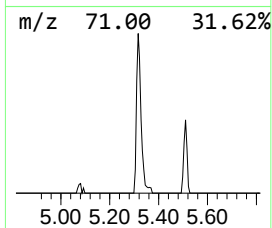
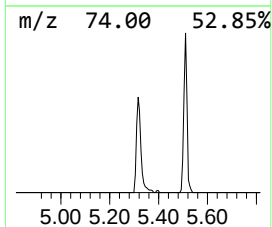
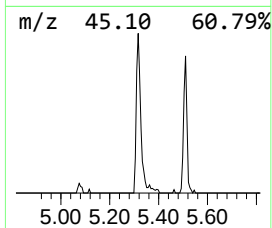
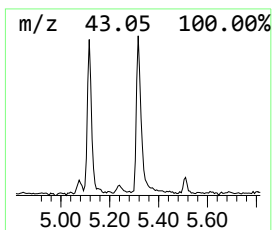
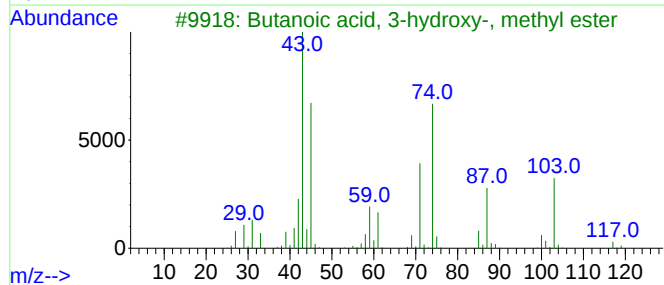
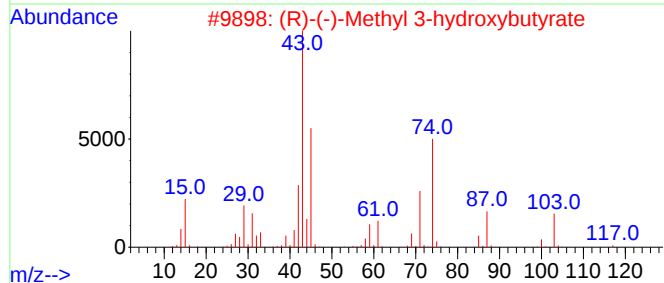
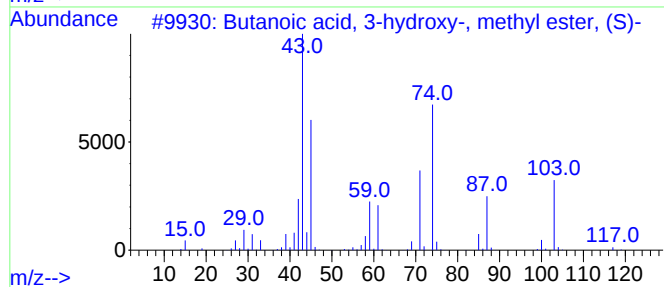
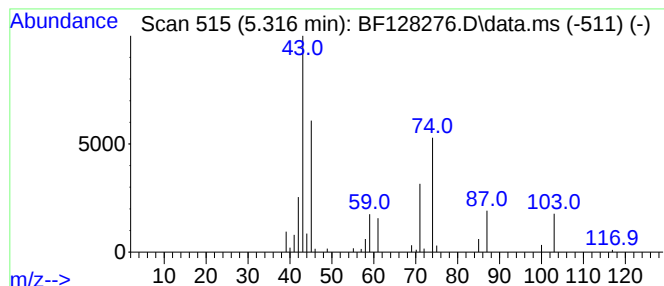
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanoic acid, 3-hydroxy-, ... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.316	3.04 ng	78633	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-hydroxy-, methy...	118	C5H10O3	053562-86-0	90
2			(R)-(-)-Methyl 3-hydroxybutyrate	118	C5H10O3	003976-69-0	90
3			Butanoic acid, 3-hydroxy-, methy...	118	C5H10O3	001487-49-6	90
4			Pentan-2-yl propyl carbonate	174	C9H18O3	1000372-82-9	32
5			Oxirane, 2-methyl-3-propyl-, cis-	100	C6H12O	006124-90-9	22



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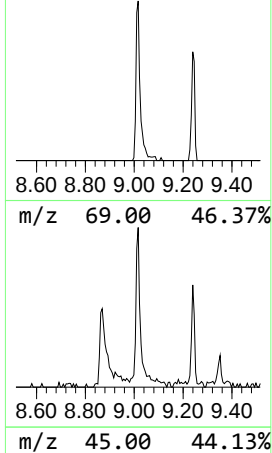
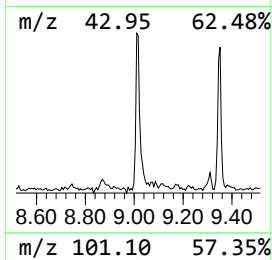
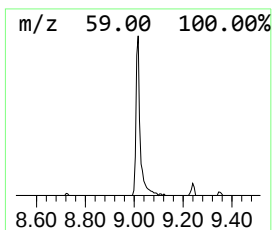
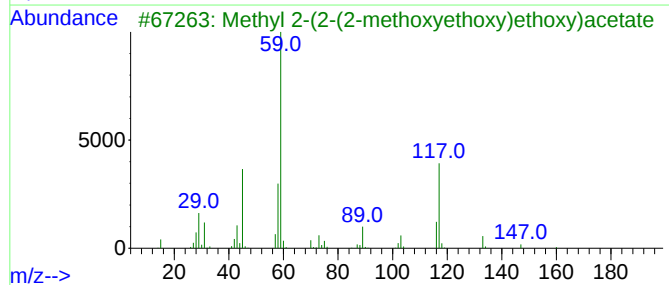
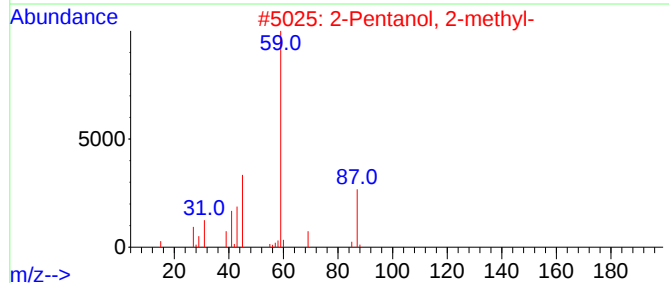
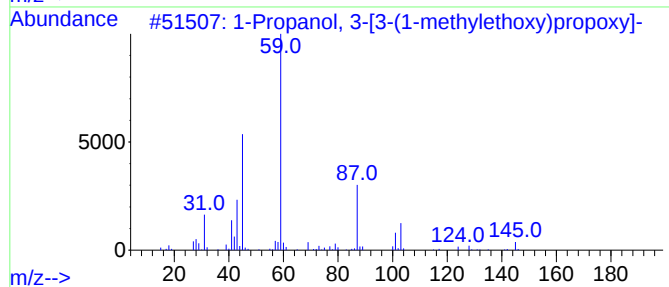
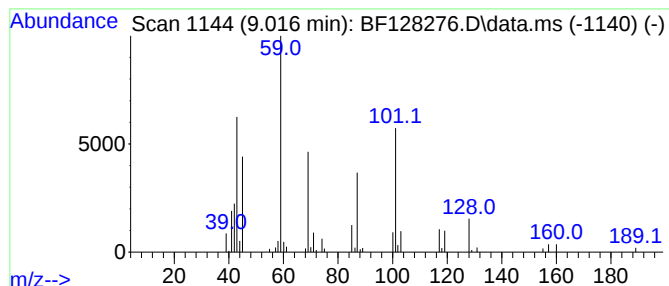
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown9.016 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.016	3.23 ng	102119	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 3-[3-(1-methylethoxy...	176	C9H20O3	054518-03-5	40		
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	38		
3	Methyl 2-(2-(2-methoxyethoxy)eth...	192	C8H16O5	1000366-88-2	37		
4	Tripropylene glycol, propyl ethe...	348	C18H40O4Si	1000367-07-2	37		
5	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	32		



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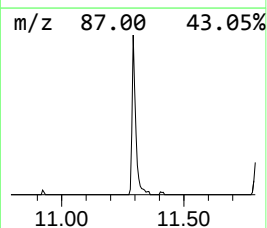
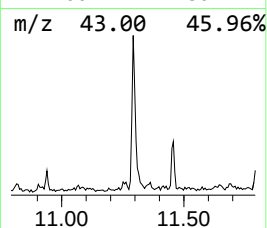
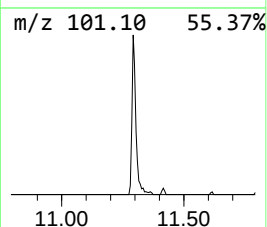
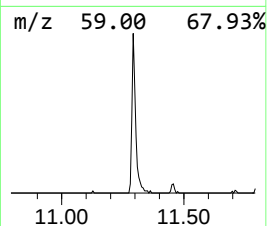
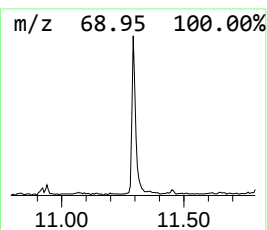
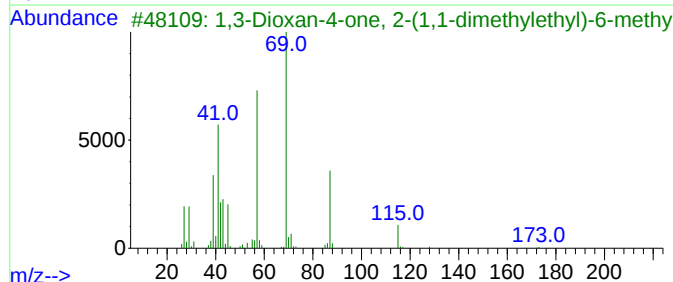
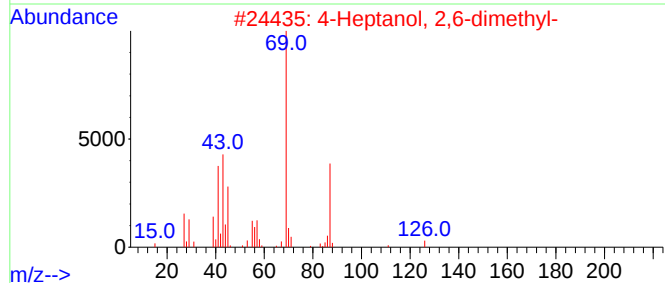
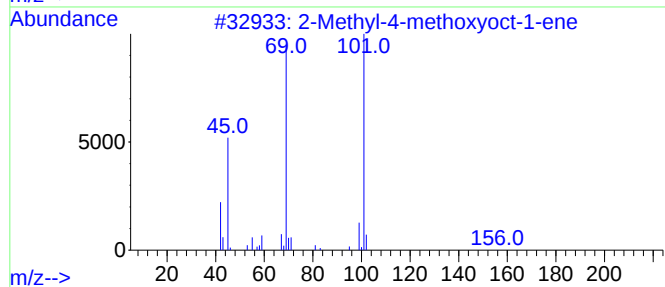
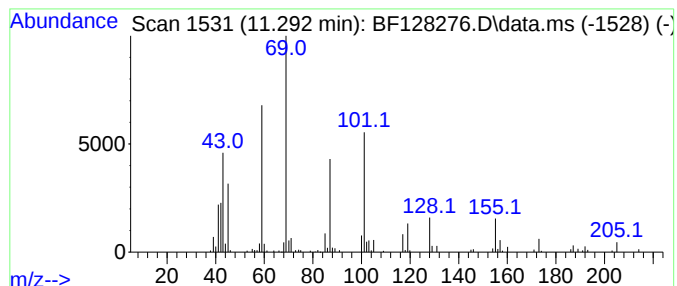
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown11.292 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.292	4.90 ng	153844	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-4-methoxyoct-1-ene	156	C10H20O	1000424-66-5	43
2			4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	38
3			1,3-Dioxan-4-one, 2-(1,1-dimethy...	172	C9H16O3	113505-75-2	37
4			3-Hexanol, 3-ethyl-	130	C8H18O	000597-76-2	35
5			1,3-Dioxan-4-one, 2-(1-methyleth...	158	C8H14O3	1000197-64-0	35



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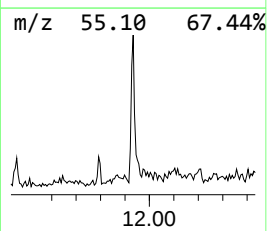
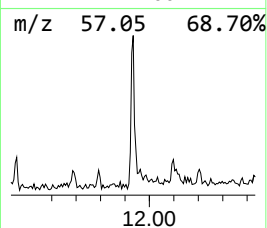
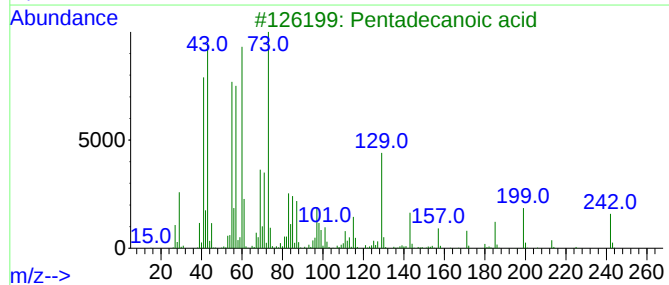
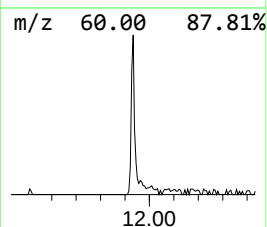
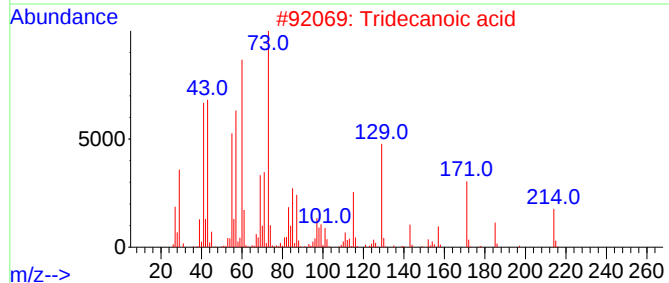
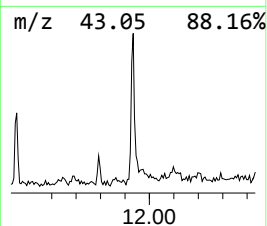
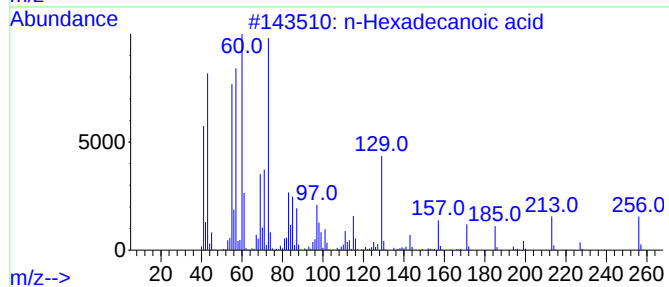
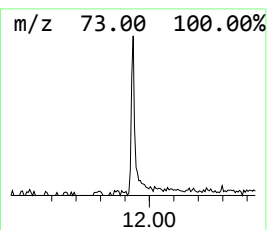
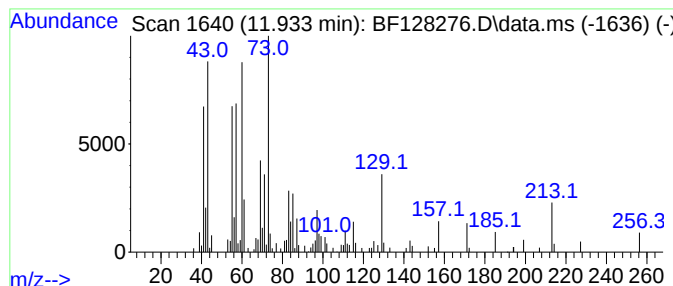
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.03 ng	95241	Phenanthrene-d10	11.416

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	43



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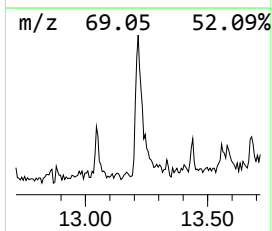
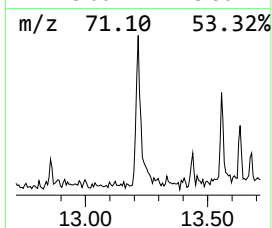
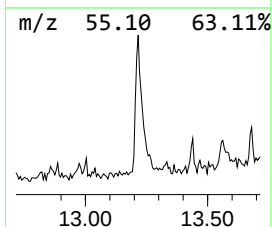
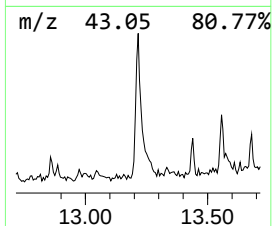
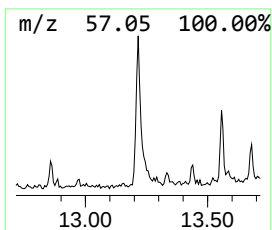
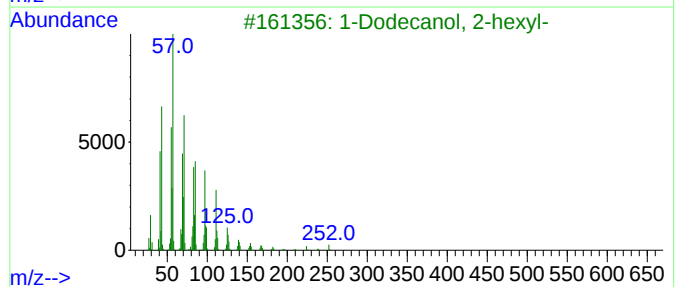
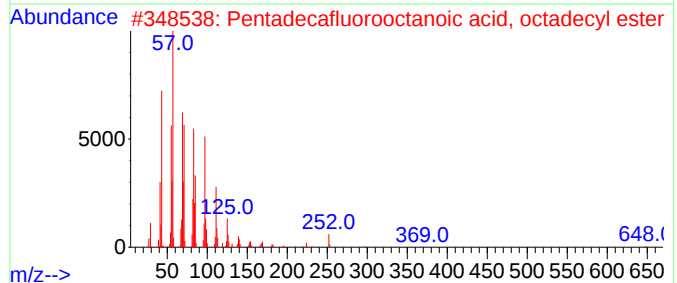
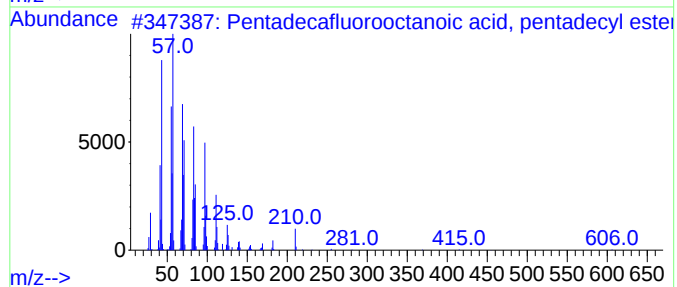
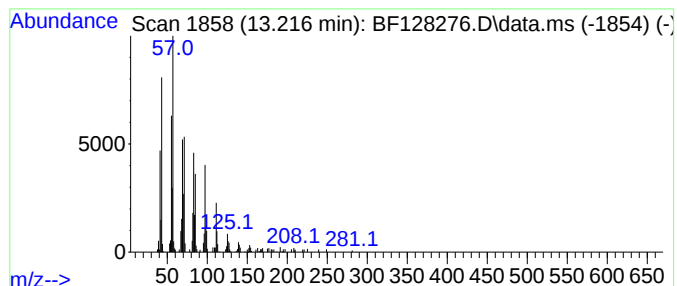
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	6.41 ng	188017	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	91
4			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
Operator : CG\JU
Sample : N2832-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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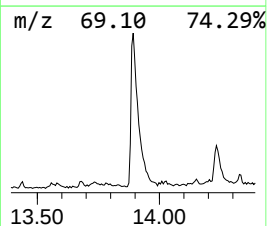
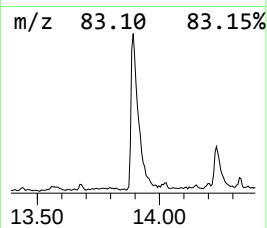
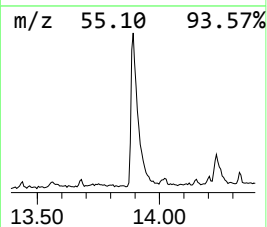
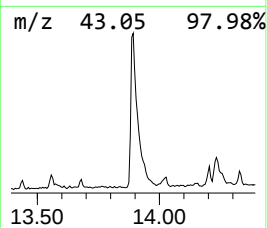
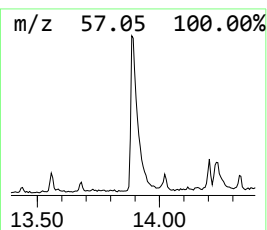
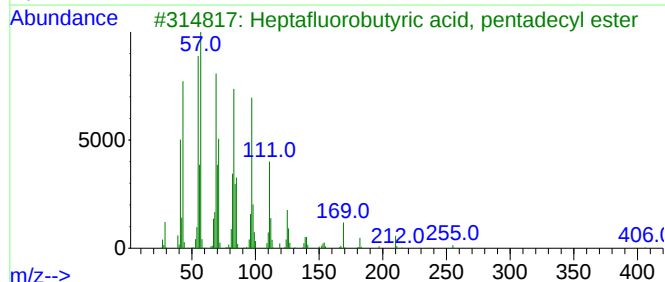
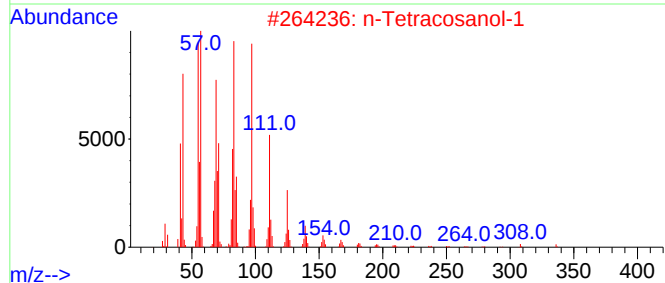
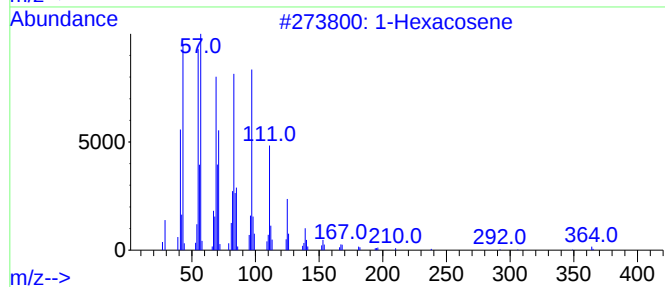
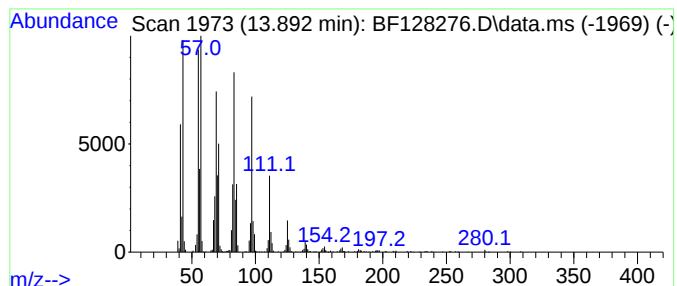
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	37.69 ng	1105780	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	94
2	n-Tetracosanol-1			354	C24H50O	000506-51-4	94
3	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	94
4	Cyclopentadecane			210	C15H30	000295-48-7	92
5	1-Heneicosanol			312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
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Acq On : 16 May 2022 19:14
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Sample : N2832-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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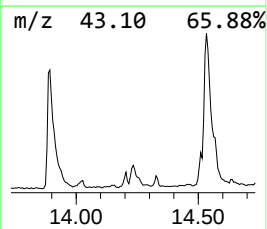
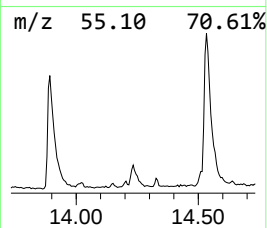
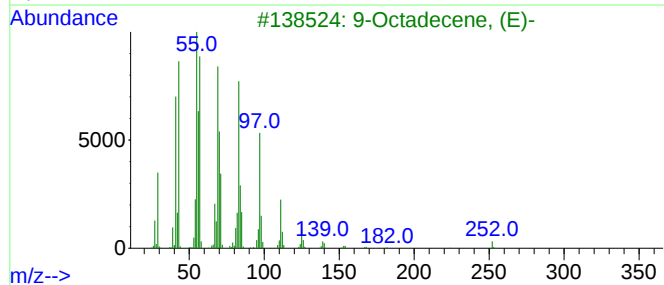
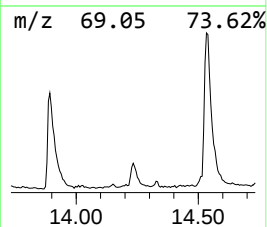
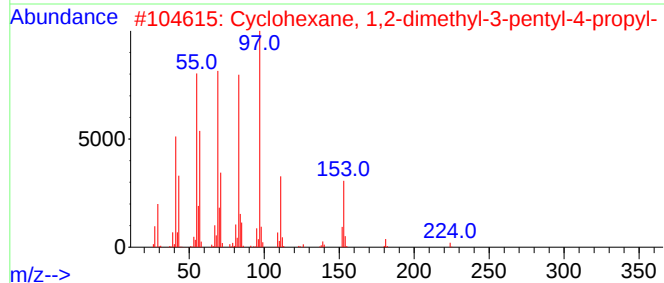
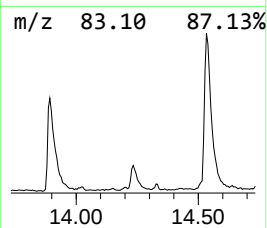
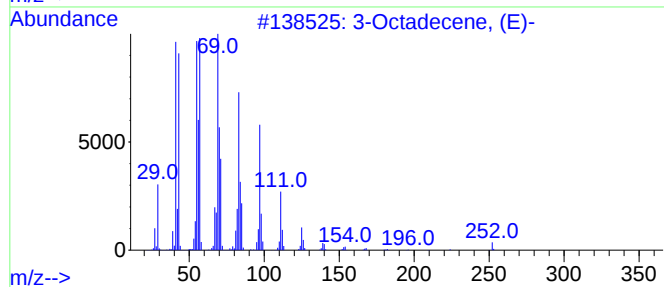
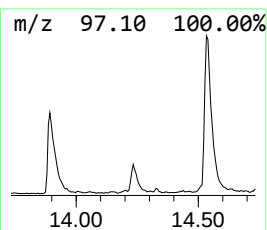
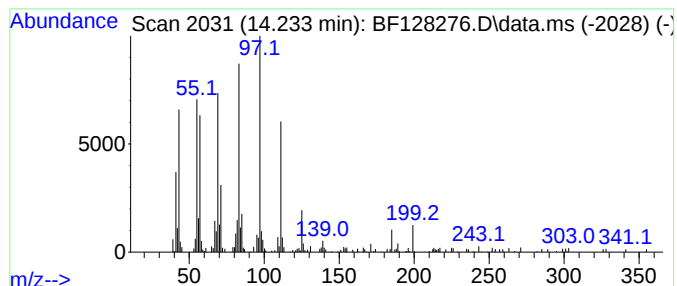
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 3-Octadecene, (E)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.233	6.08 ng	178498	Chrysene-d12	14.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Octadecene, (E)-	252	C18H36	007206-19-1	86
2		Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	72
3		9-Octadecene, (E)-	252	C18H36	007206-25-9	50
4		2-Thiopheneacetic acid, 3,5-dime...	252	C14H20O2S	1000278-92-2	41
5		Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
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Sample : N2832-08
Misc :
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Instrument :
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ClientSampleId :
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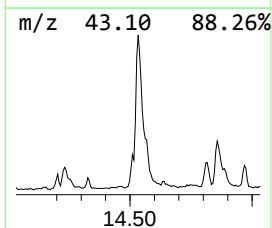
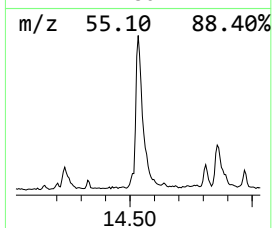
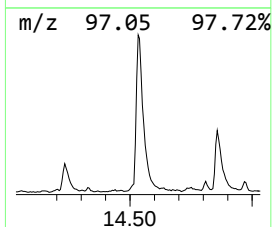
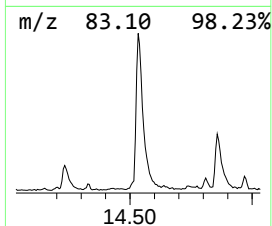
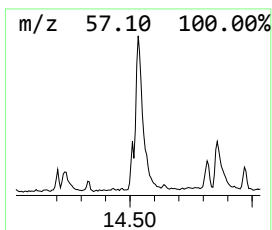
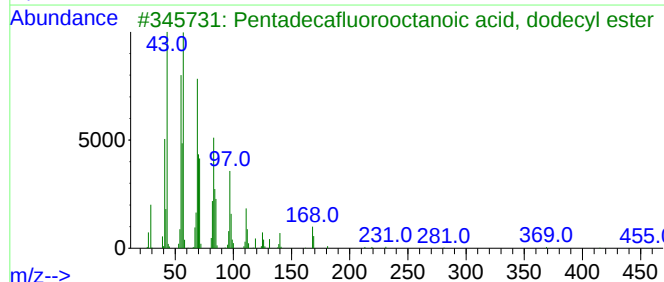
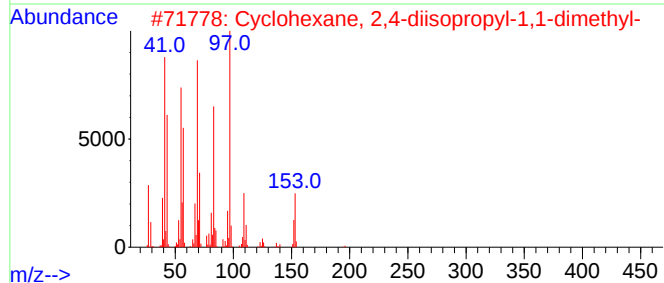
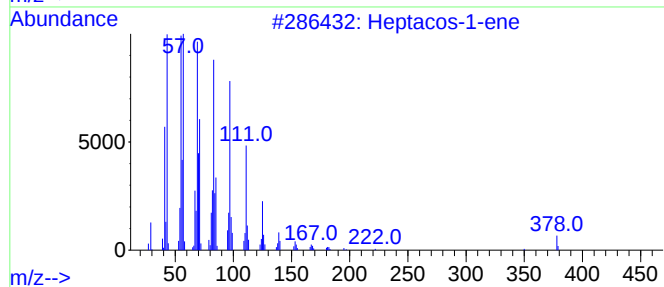
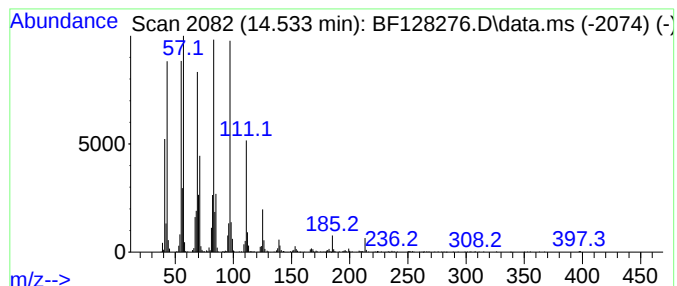
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Heptacos-1-ene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	60.71 ng	1780900	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacos-1-ene	378	C27H54	015306-27-1	64
2			Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	58
3			Pentadecafluorooctanoic acid, do...	582	C20H25F15O2	1000406-04-2	53
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	50
5			Octacosanol	410	C28H58O	000557-61-9	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
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Misc :
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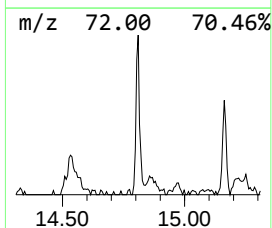
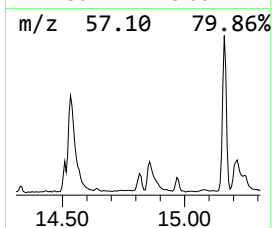
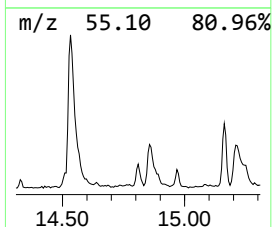
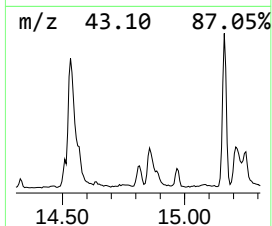
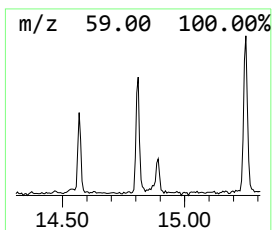
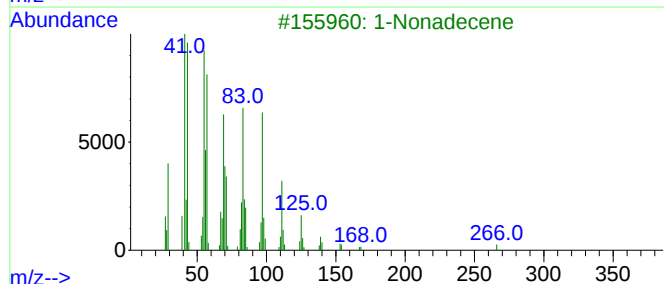
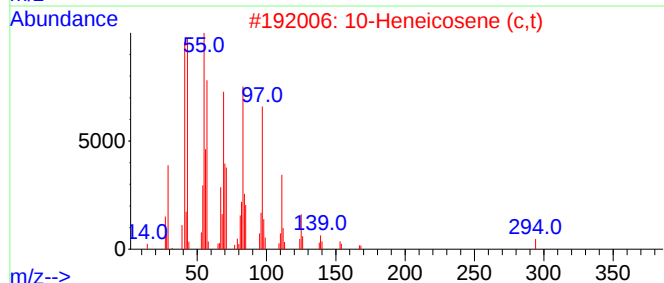
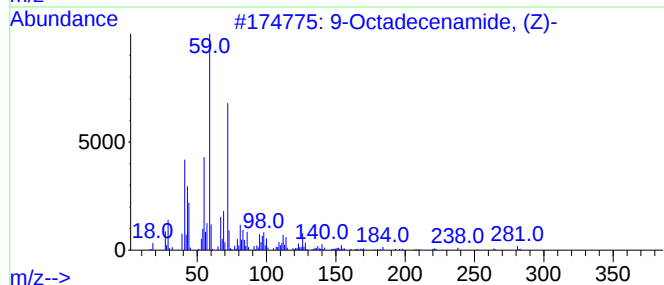
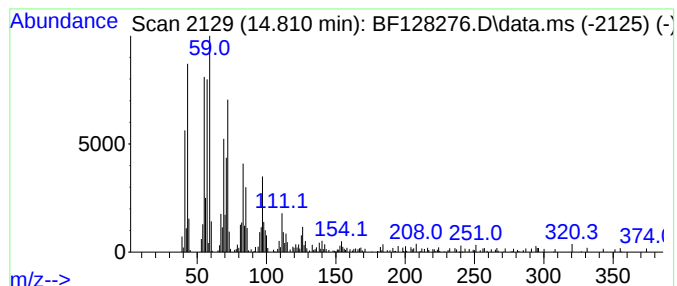
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.810	5.74 ng	168367	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	10-Heneicosene (c,t)	294	C21H42	095008-11-0	53
3	1-Nonadecene	266	C19H38	018435-45-5	46
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	46
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
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Sample : N2832-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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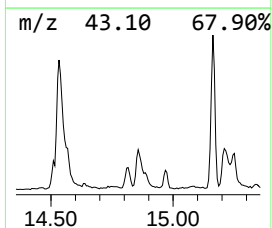
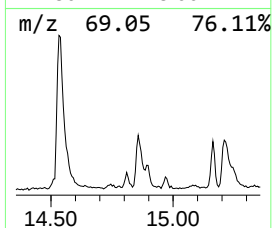
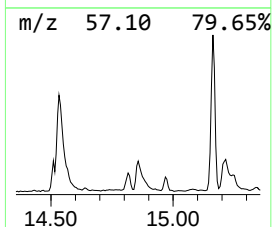
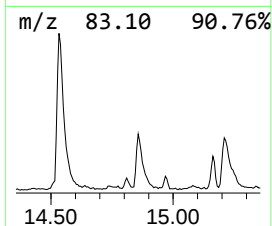
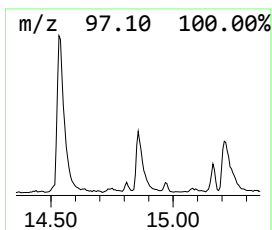
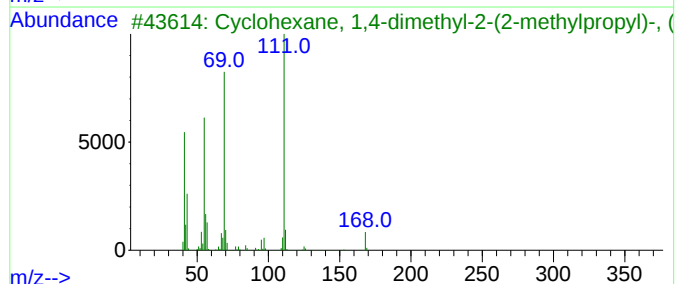
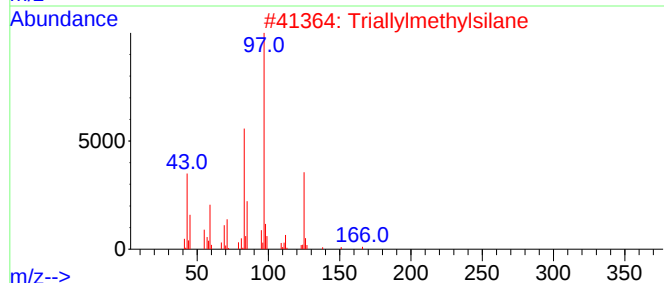
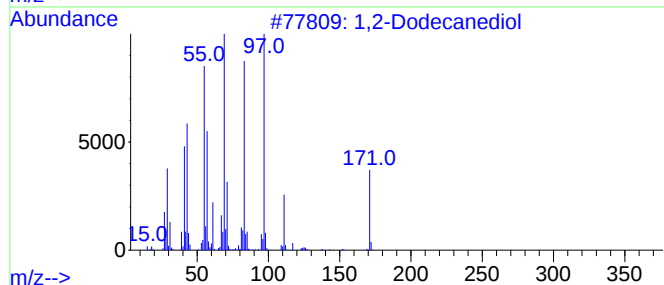
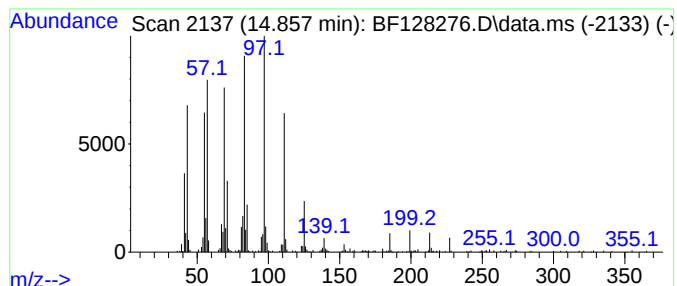
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1,2-Dodecanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	23.53 ng	545134	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dodecanediol	202	C12H26O2	001119-87-5	72
2			Triallylmethylsilane	166	C10H18Si	001112-91-0	38
3			Cyclohexane, 1,4-dimethyl-2-(2-m...	168	C12H24	054411-17-5	30
4			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	25
5			3-Amino-2-cyclohexenone	111	C6H9NO	005220-49-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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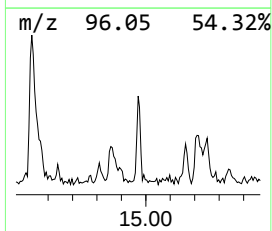
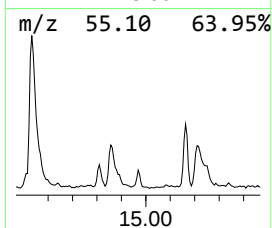
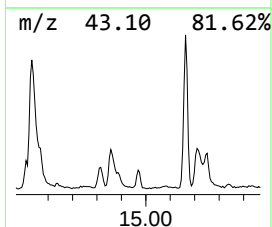
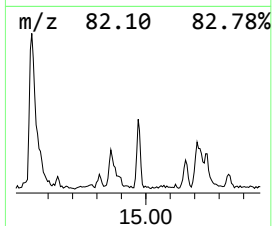
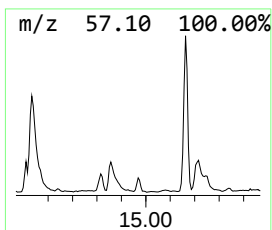
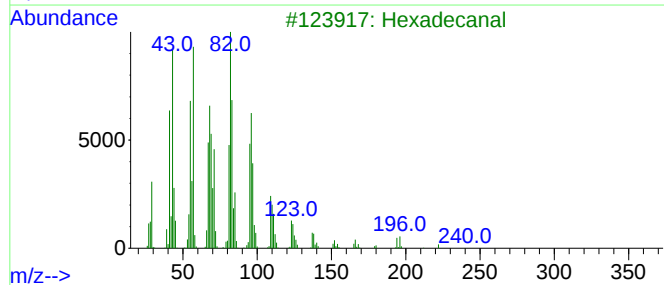
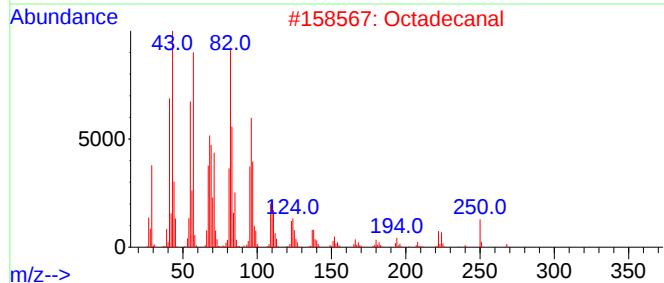
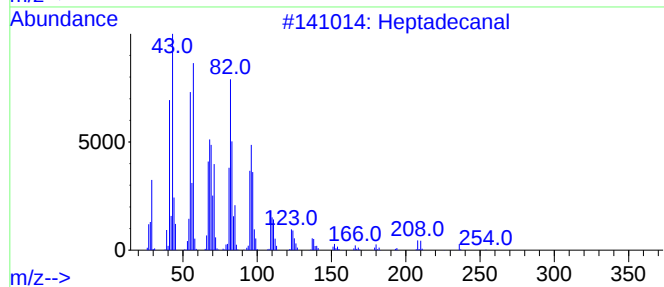
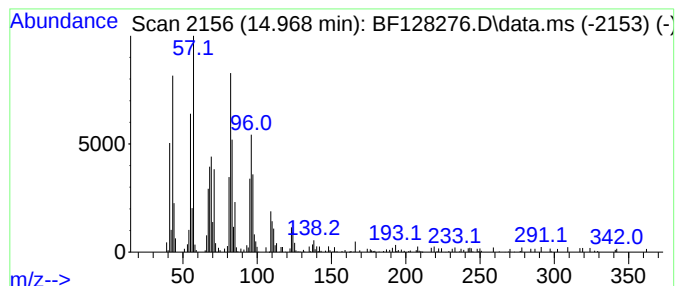
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heptadecanal Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	5.00 ng	115822	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanal	254	C17H34O	1000376-70-0	91
2			Octadecanal	268	C18H36O	000638-66-4	91
3			Hexadecanal	240	C16H32O	000629-80-1	91
4			Eicosanal-	296	C20H40O	002400-66-0	91
5			17-Octadecenal	266	C18H34O	056554-86-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
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Sample : N2832-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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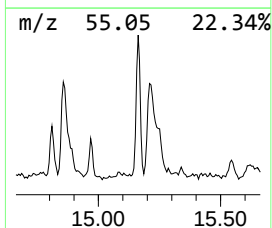
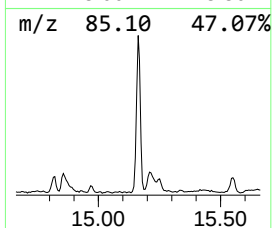
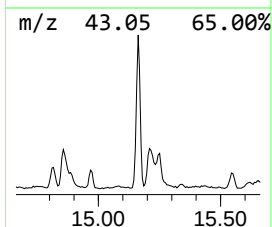
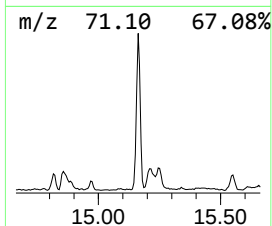
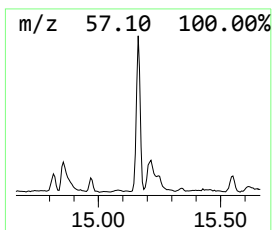
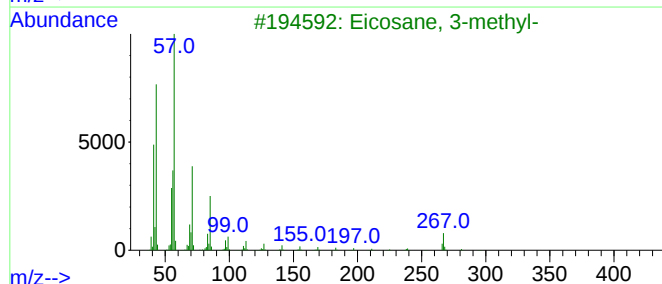
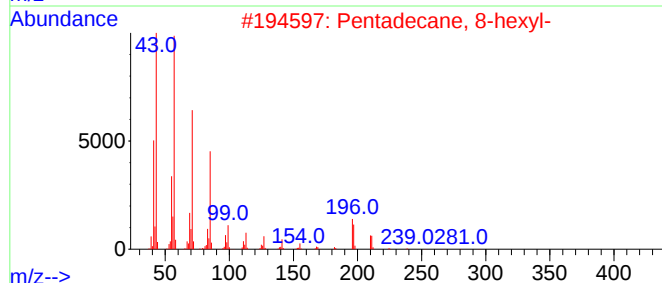
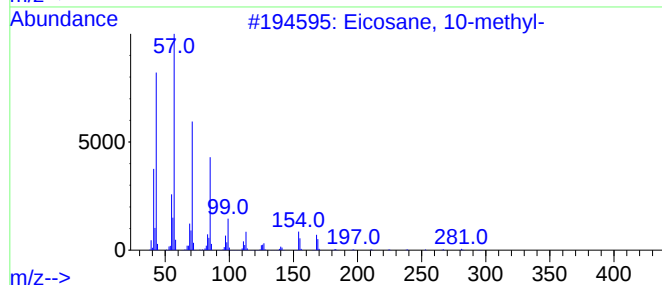
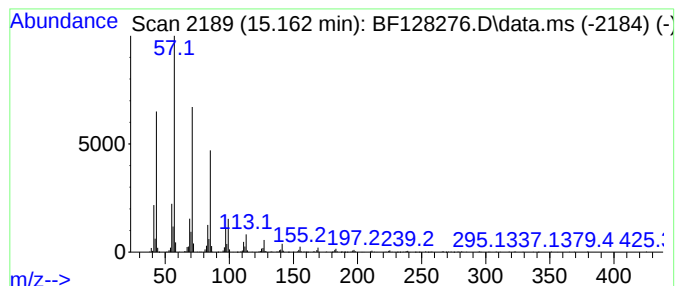
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Eicosane, 10-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	28.27 ng	654934	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
2			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
3			Eicosane, 3-methyl-	296	C21H44	006418-46-8	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
Operator : CG\JU
Sample : N2832-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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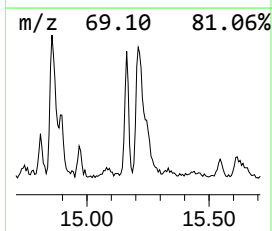
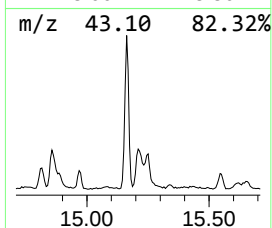
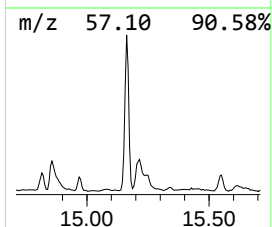
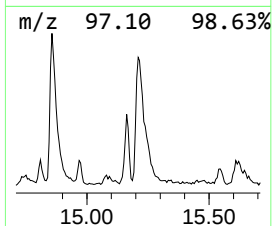
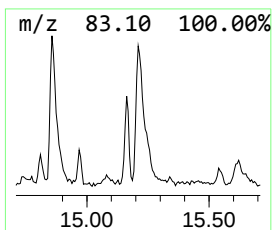
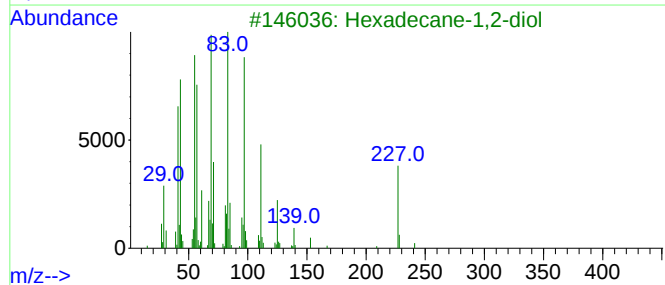
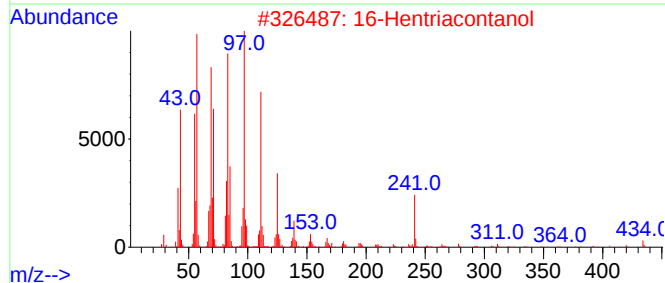
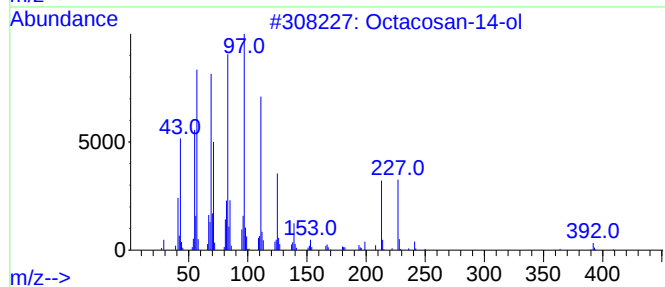
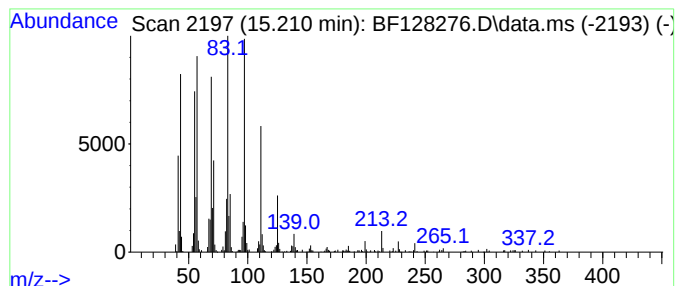
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octacosan-14-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	20.97 ng	485977	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosan-14-ol	410	C28H58O	138967-02-9	91
2			16-Hentriacontanol	452	C31H64O	001070-54-8	87
3			Hexadecane-1,2-diol	258	C16H34O2	006920-24-7	86
4			Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	50
5			Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
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Sample : N2832-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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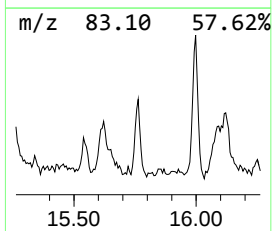
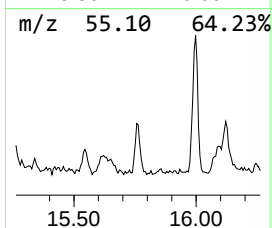
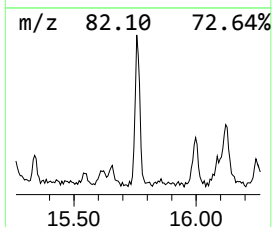
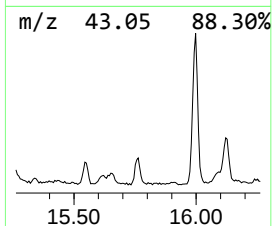
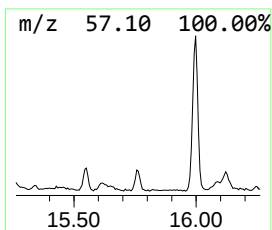
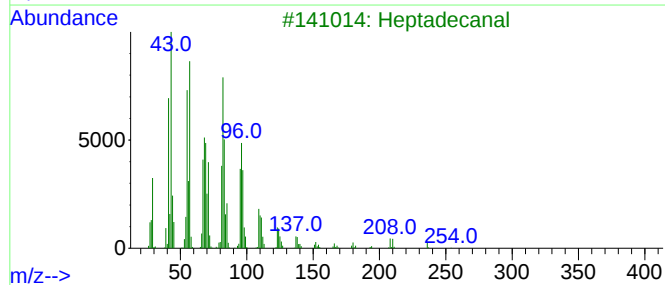
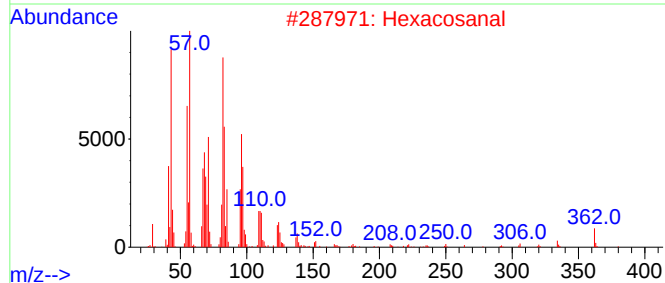
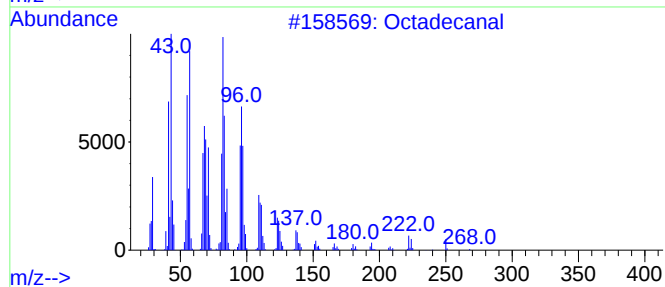
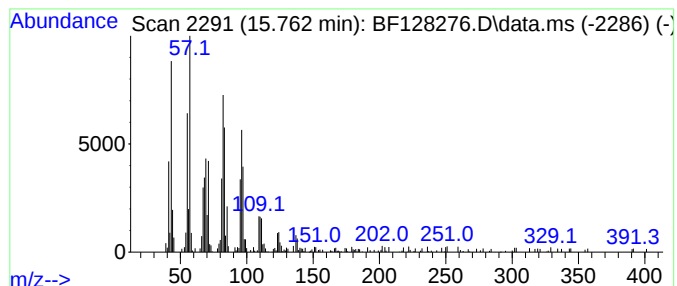
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Octadecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.762	7.80 ng	180660	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	98
2			Hexacosanal	380	C26H52O	026627-85-0	95
3			Heptadecanal	254	C17H34O	1000376-70-0	91
4			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
5			Octacosanal	408	C28H56O	022725-64-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
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Sample : N2832-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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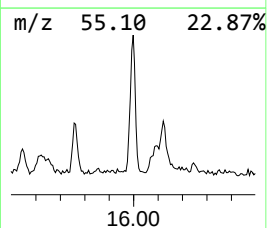
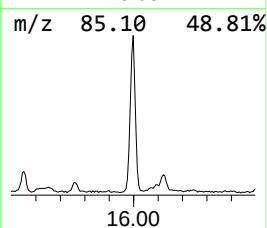
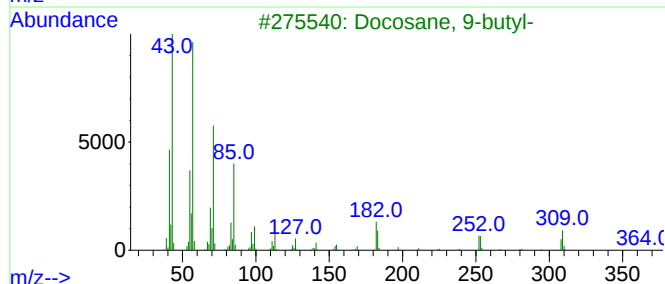
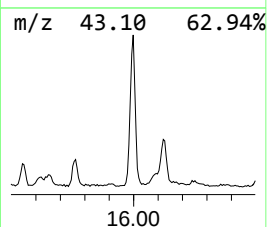
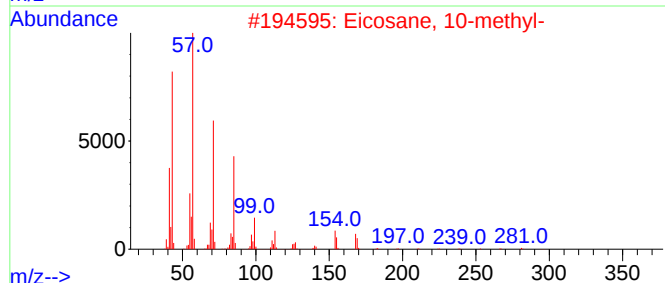
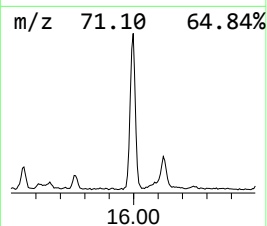
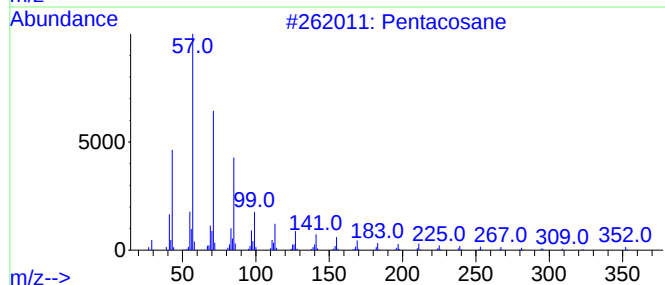
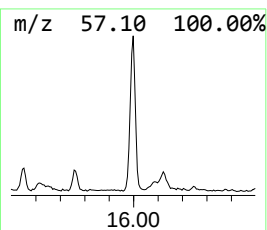
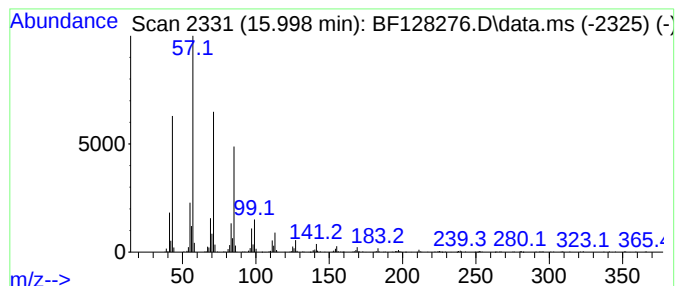
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	26.20 ng	607087	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	97
2			Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
3			Docosane, 9-butyl-	366	C26H54	055282-14-9	94
4			Docosane, 5-butyl-	366	C26H54	055282-16-1	93
5			2-Methylpentacosane	366	C26H54	000629-87-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
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Sample : N2832-08
Misc :
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Instrument :
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ClientSampleId :
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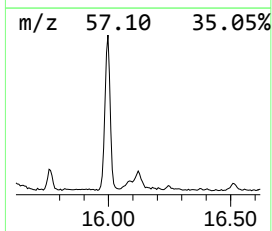
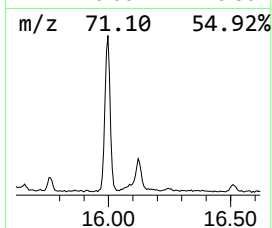
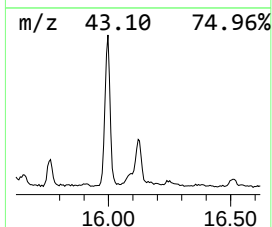
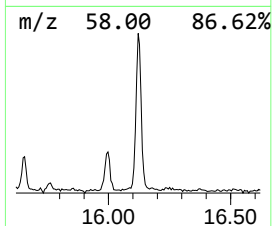
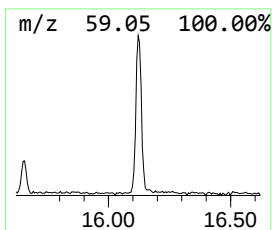
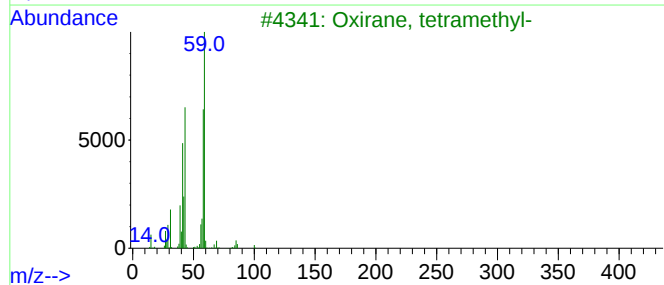
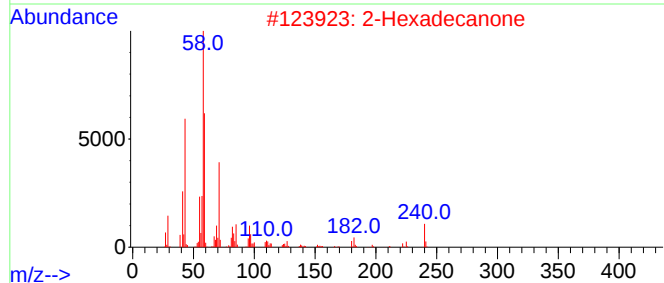
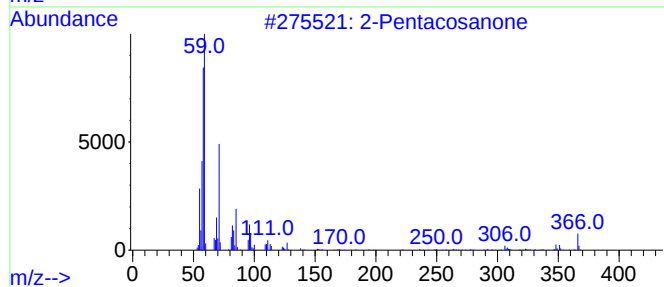
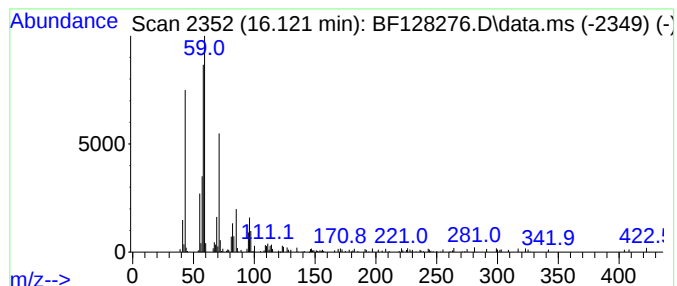
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 2-Pentacosanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.121	9.50 ng	220056	Perylene-d12	15.557

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentacosanone	366	C25H50O	075207-54-4	83
2		2-Hexadecanone	240	C16H32O	018787-63-8	64
3		Oxirane, tetramethyl-	100	C6H12O	005076-20-0	50
4		2-Tetradecanone	212	C14H28O	002345-27-9	43
5		D-Ribose, 5-O-methyl-2,3-O-(1-me...	204	C9H16O5	064018-53-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
Operator : CG\JU
Sample : N2832-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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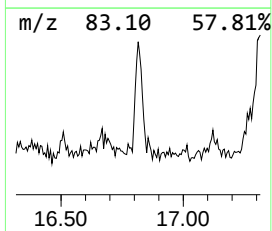
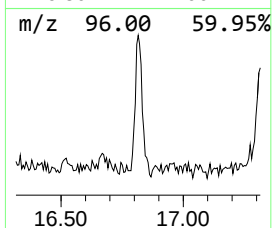
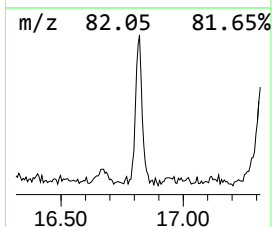
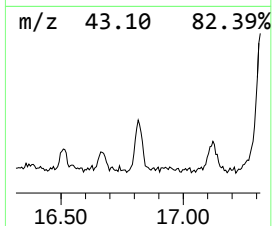
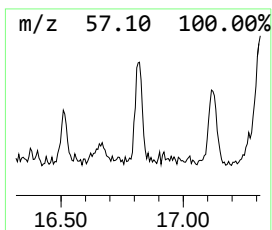
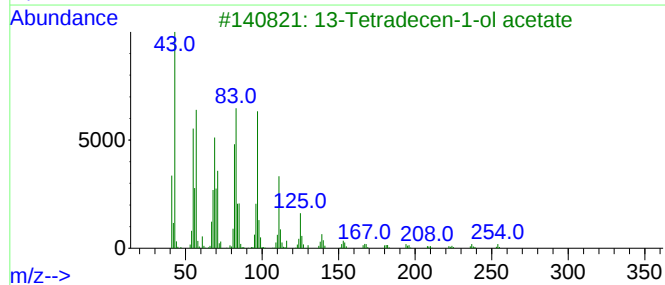
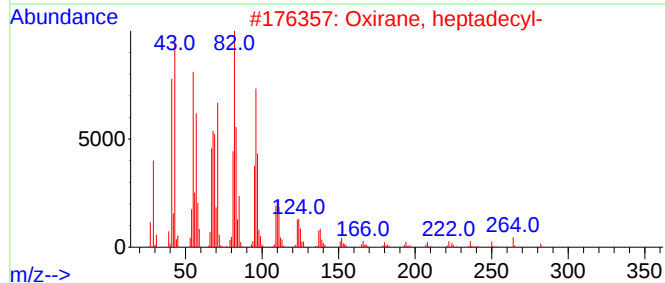
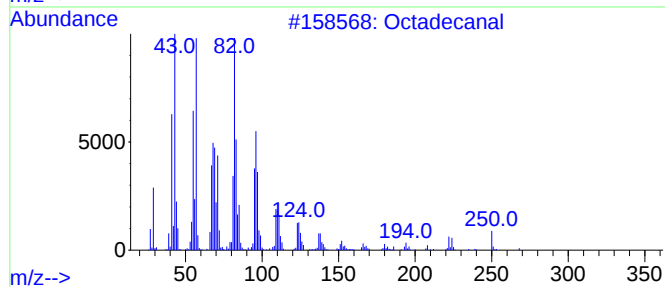
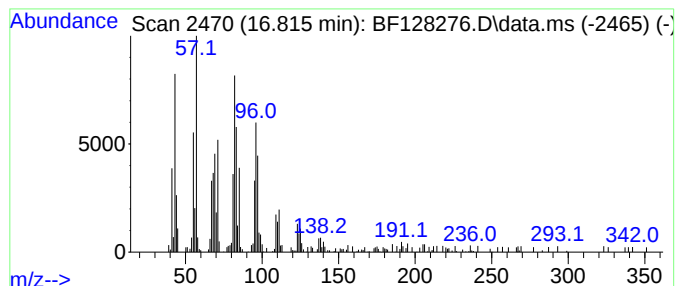
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Oxirane, heptadecyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.815	6.95 ng	161087	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	87
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	70
3			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	64
4			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	60
5			1,19-Eicosadiene	278	C20H38	014811-95-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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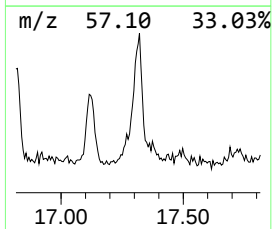
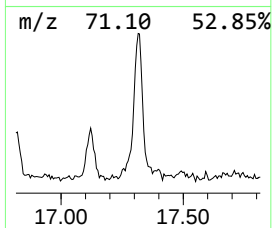
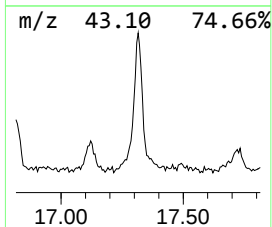
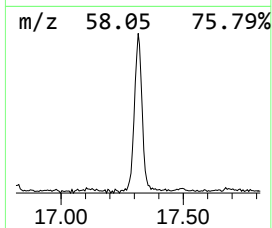
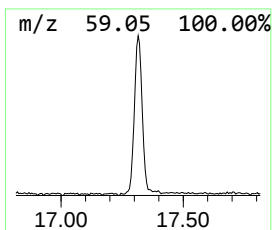
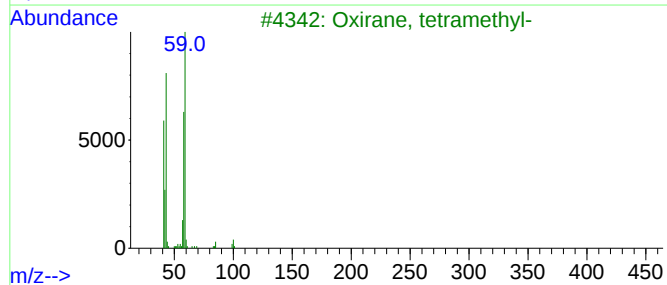
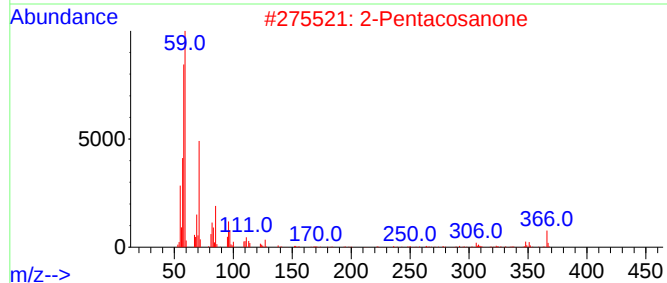
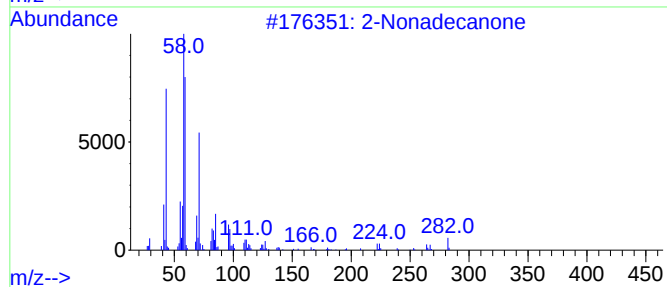
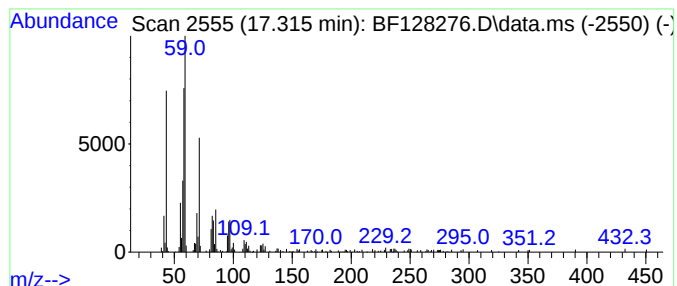
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 2-Nonadecanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.315	8.28 ng	191801	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonadecanone			282	C19H38O	000629-66-3	59
2	2-Pentacosanone			366	C25H50O	075207-54-4	56
3	Oxirane, tetramethyl-			100	C6H12O	005076-20-0	50
4	9-Decen-2-one			154	C10H18O	035194-30-0	38
5	2,3-Butanediol, 1,4-dibromo-2,3-...			274	C6H12Br2O2	1010142-97-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
Operator : CG\JU
Sample : N2832-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB10

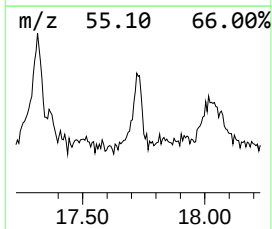
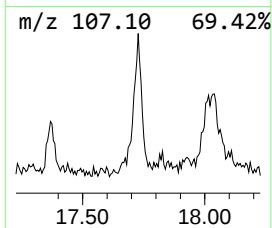
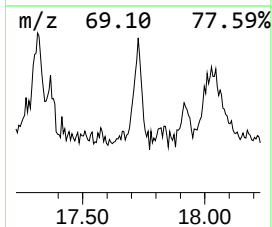
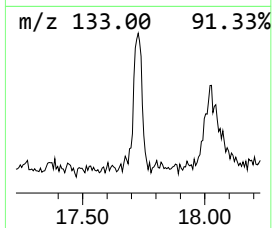
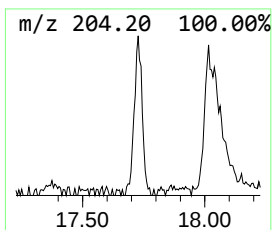
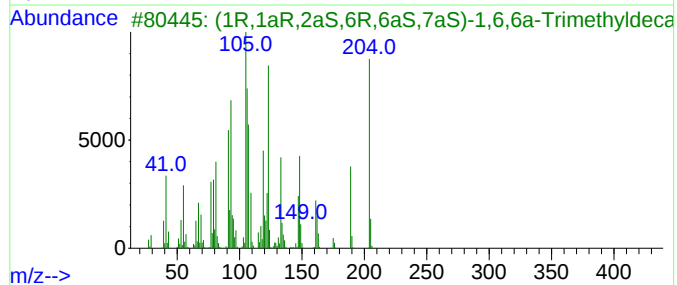
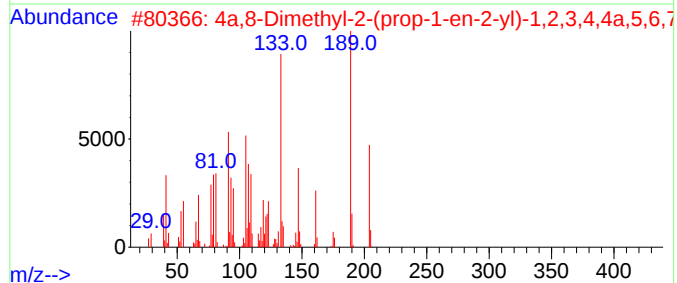
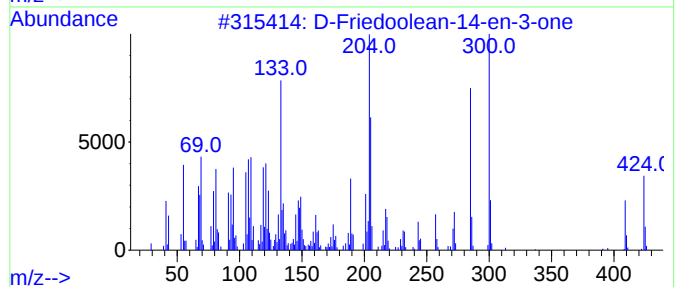
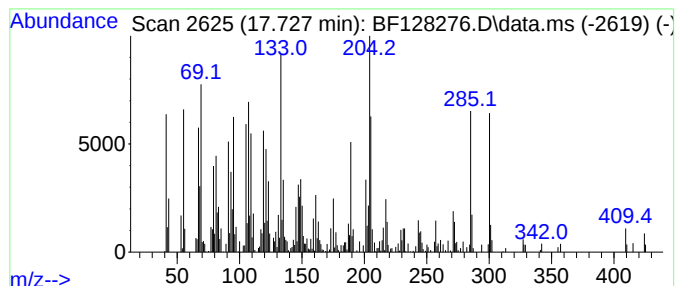
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 D-Friedoolean-14-en-3-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	15.05 ng	348655	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Friedoolean-14-en-3-one	424	C30H48O	000514-07-8	99
2			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	70
3			(1R,1aR,2aS,6R,6aS,7aS)-1,6,6a-T...	204	C15H24	026620-70-2	49
4			cis-Thujopsene	204	C15H24	000470-40-6	46
5			Himachala-2,4-diene	204	C15H24	060909-27-5	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128276.D
Acq On : 16 May 2022 19:14
Operator : CG\JU
Sample : N2832-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB10

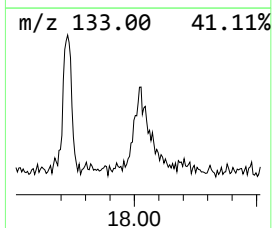
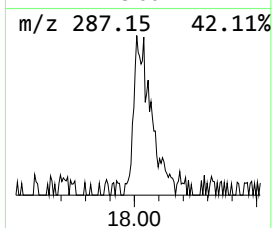
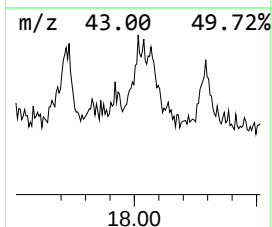
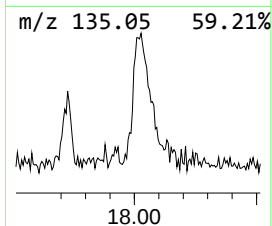
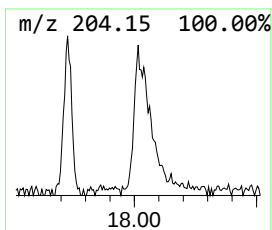
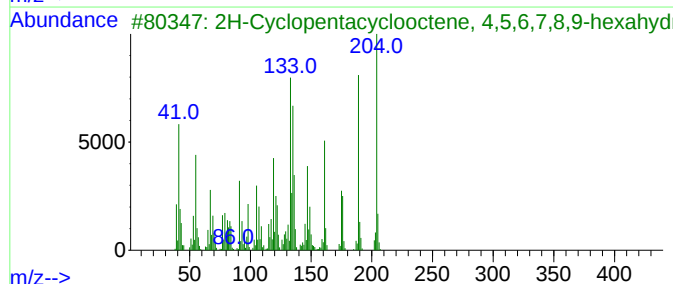
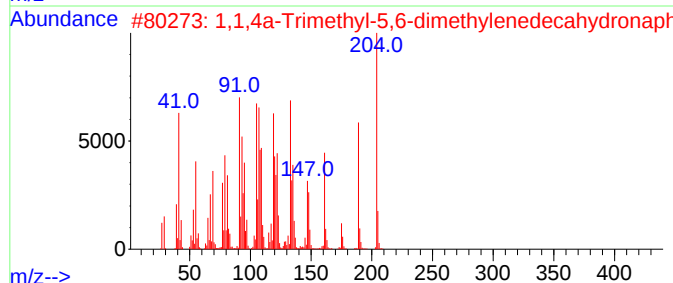
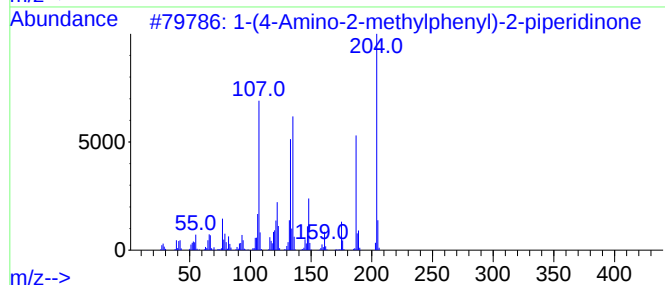
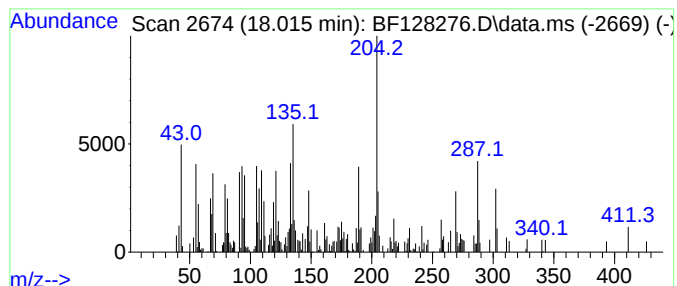
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 1-(4-Amino-2-methylphenyl)-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.015	18.69 ng	433057	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Amino-2-methylphenyl)-2-pip...	204	C12H16N2O	443999-53-9	55		
2	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	50		
3	2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	49		
4	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	49		
5	3-Chloro-5-fluoro-4-methoxybenzo...	204	C8H6ClFO3	886497-22-9	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
 Data File : BF128276.D
 Acq On : 16 May 2022 19:14
 Operator : CG\JU
 Sample : N2832-08
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid, ...	5.316	3.0	ng	78633	1	6.887	517698	20.0
unknown9.016	9.016	3.2	ng	102119	2	8.169	632238	20.0
unknown11.292	11.292	4.9	ng	153844	4	11.416	628433	20.0
n-Hexadecanoic ...	11.933	3.0	ng	95241	4	11.416	628433	20.0
Pentadecafluoro...	13.216	6.4	ng	188017	5	14.063	586732	20.0
1-Hexacosene	13.892	37.7	ng	1105780	5	14.063	586732	20.0
3-Octadecene, (E)-	14.233	6.1	ng	178498	5	14.063	586732	20.0
Heptacos-1-ene	14.533	60.7	ng	1780900	5	14.063	586732	20.0
9-Octadecenamid...	14.810	5.7	ng	168367	5	14.063	586732	20.0
1,2-Dodecanediol	14.857	23.5	ng	545134	6	15.557	463402	20.0
Heptadecanal	14.968	5.0	ng	115822	6	15.557	463402	20.0
Eicosane, 10-me...	15.163	28.3	ng	654934	6	15.557	463402	20.0
Octacosan-14-ol	15.210	21.0	ng	485977	6	15.557	463402	20.0
Octadecanal	15.762	7.8	ng	180660	6	15.557	463402	20.0
Pentacosane	15.998	26.2	ng	607087	6	15.557	463402	20.0
2-Pentacosanone	16.121	9.5	ng	220056	6	15.557	463402	20.0
Oxirane, heptad...	16.815	7.0	ng	161087	6	15.557	463402	20.0
2-Nonadecanone	17.315	8.3	ng	191801	6	15.557	463402	20.0
D-Friedoolean-1...	17.727	15.1	ng	348655	6	15.557	463402	20.0
1-(4-Amino-2-me...	18.015	18.7	ng	433057	6	15.557	463402	20.0