

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
 Data File : BF136834.D
 Acq On : 29 Dec 2023 17:44
 Operator : CG\JU
 Sample : 05897-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-36a

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136834.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.899	133	138	146	rVB	36626	57627	2.87%	0.414%
2	3.352	212	215	233	rBV	33871	75379	3.76%	0.542%
3	5.034	497	501	508	rVB	26865	34723	1.73%	0.250%
4	5.428	564	568	571	rBV	1855391	1655407	82.56%	11.895%
5	6.428	733	738	741	rBV	1643705	1671348	83.36%	12.010%
6	6.781	794	798	802	rBV	515431	398313	19.87%	2.862%
7	7.345	889	894	897	rBV	1235361	1106186	55.17%	7.949%
8	7.598	933	937	945	rBV	24786	21829	1.09%	0.157%
9	8.057	1011	1015	1018	rBV	658808	520322	25.95%	3.739%
10	8.375	1066	1069	1080	rBV	24184	42958	2.14%	0.309%
11	9.134	1193	1198	1202	rBV	2169006	2005035	100.00%	14.408%
12	9.816	1310	1314	1317	rBV	673007	587560	29.30%	4.222%
13	9.916	1326	1331	1339	rVB2	26325	38482	1.92%	0.277%
14	10.610	1445	1449	1452	rBV	1314272	1171411	58.42%	8.418%
15	11.304	1564	1567	1571	rBV	698141	605050	30.18%	4.348%
16	11.839	1655	1658	1673	rBV	196184	263416	13.14%	1.893%
17	12.092	1697	1701	1704	rBV	42747	34640	1.73%	0.249%
18	12.633	1790	1793	1806	rBV3	31685	62913	3.14%	0.452%
19	12.904	1834	1839	1842	rBV	1971690	1714598	85.51%	12.321%
20	13.133	1873	1878	1881	rBV	29737	25032	1.25%	0.180%
21	13.480	1932	1937	1940	rVB2	26064	31828	1.59%	0.229%
22	13.810	1989	1993	1997	rBV	237937	192457	9.60%	1.383%
23	13.886	1997	2006	2012	rBV10	24954	86931	4.34%	0.625%
24	13.963	2015	2019	2025	rVB	429162	402173	20.06%	2.890%
25	14.127	2042	2047	2050	rVB2	34328	34885	1.74%	0.251%
26	14.433	2095	2099	2103	rBV	165406	159286	7.94%	1.145%
27	14.745	2147	2152	2156	rVB2	21758	28415	1.42%	0.204%
28	14.892	2174	2177	2180	rVB3	23434	23341	1.16%	0.168%
29	15.086	2206	2210	2215	rVB	71287	79861	3.98%	0.574%
30	15.168	2221	2224	2228	rBV	22118	25890	1.29%	0.186%
31	15.445	2265	2271	2280	rBV	276457	380861	19.00%	2.737%
32	15.680	2308	2311	2316	rVB7	19348	27552	1.37%	0.198%
33	15.921	2347	2352	2358	rVB	49595	74815	3.73%	0.538%
34	16.051	2366	2374	2384	rBV6	30081	79860	3.98%	0.574%
35	16.704	2479	2485	2489	rBV8	14752	30967	1.54%	0.223%
36	16.745	2489	2492	2499	rVB8	17365	30029	1.50%	0.216%

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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-BF122023.M
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37	17.057	2540	2545	2552	rVB4	17740	36127	1.80%	0.260%
38	17.798	2663	2671	2679	rVB9	38755	98783	4.93%	0.710%

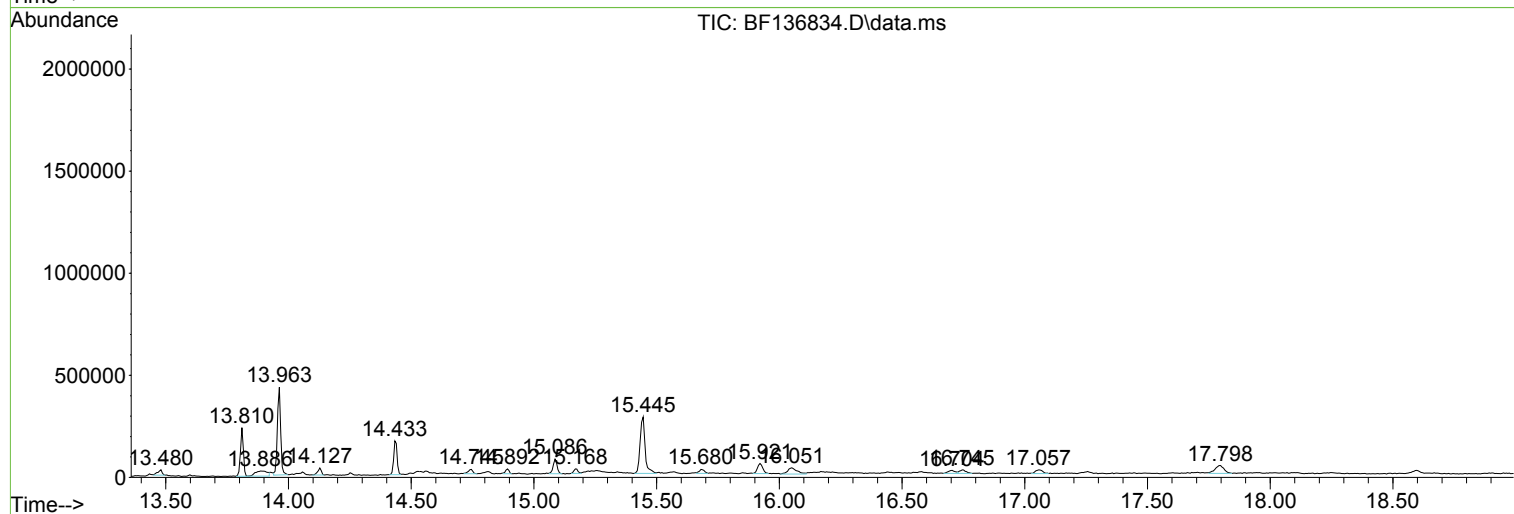
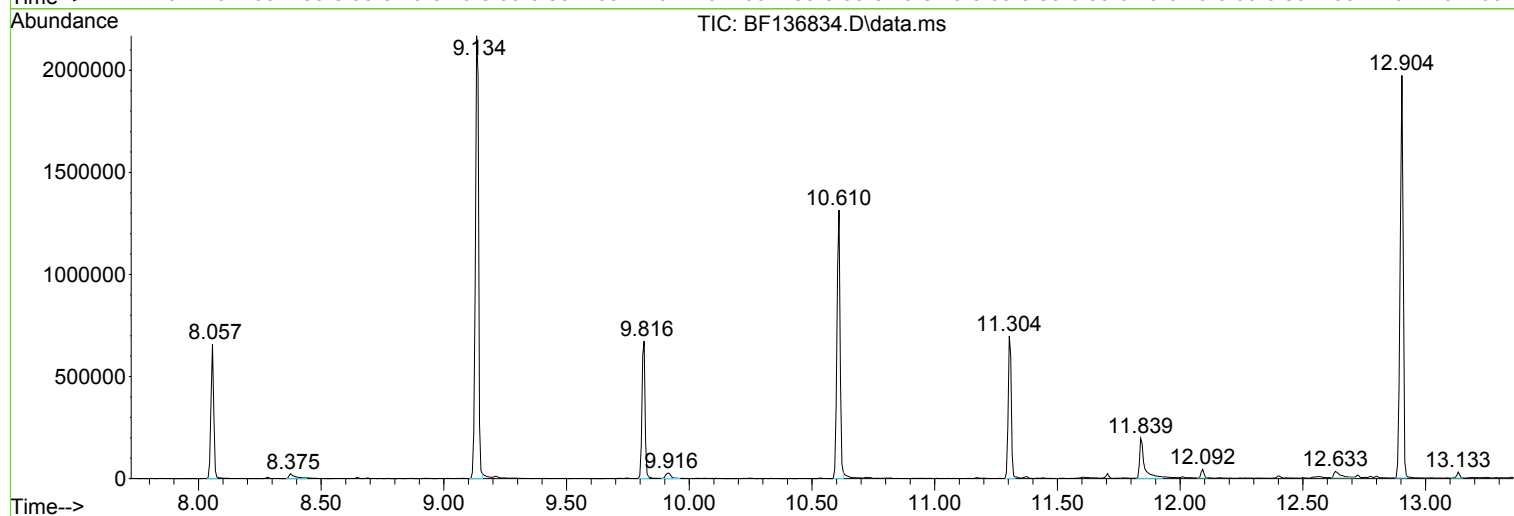
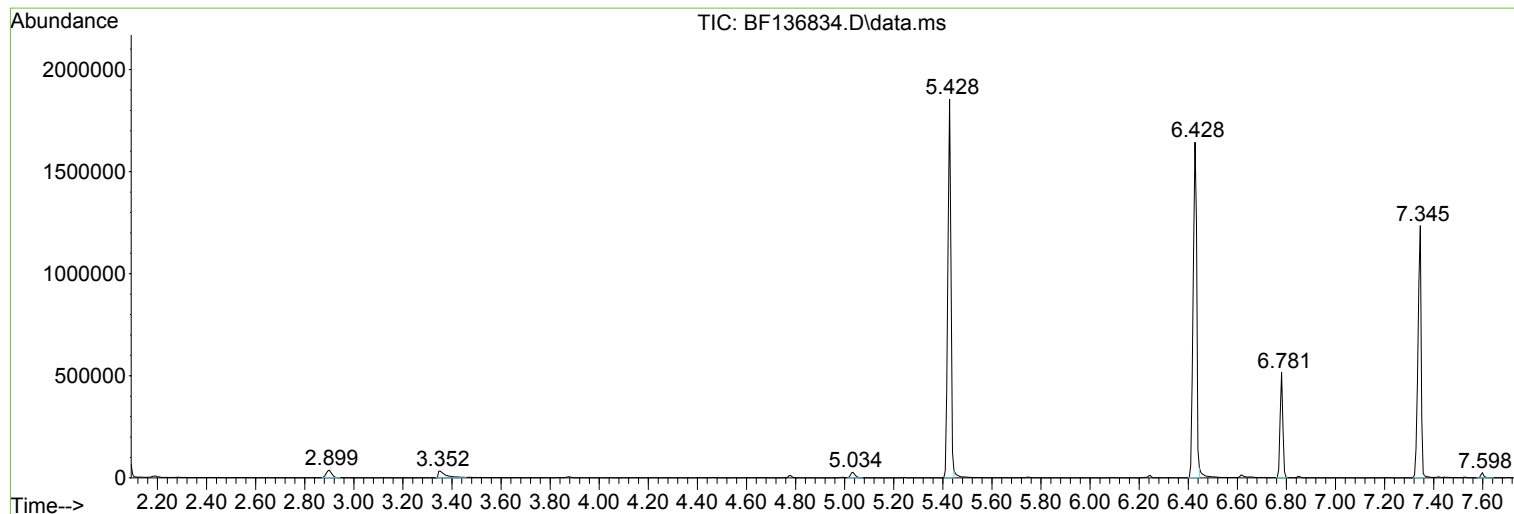
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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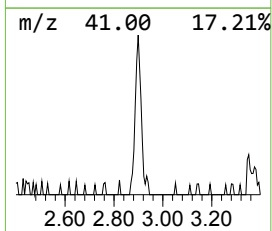
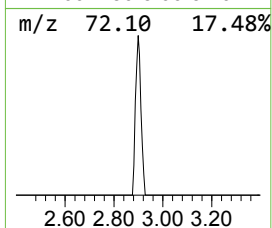
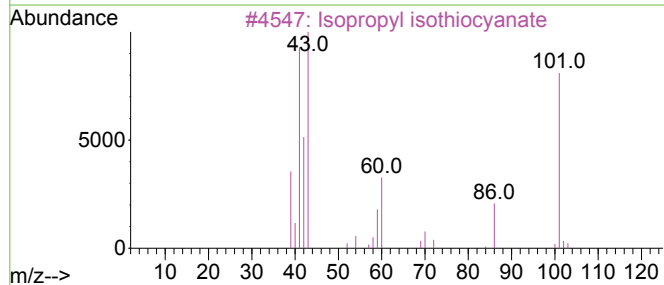
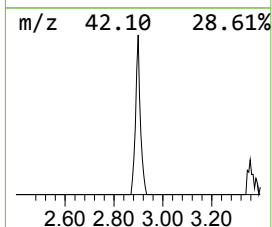
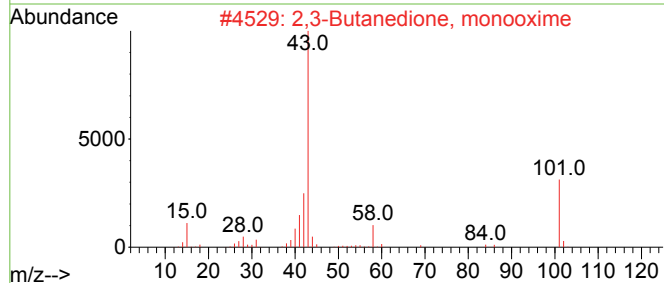
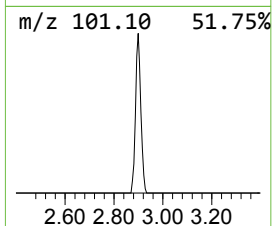
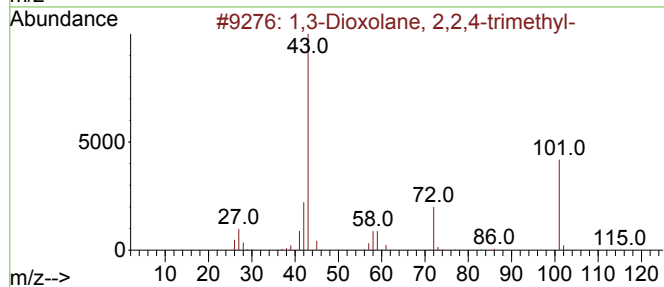
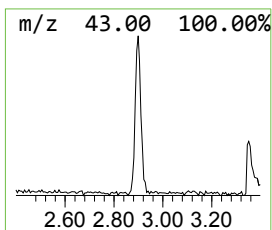
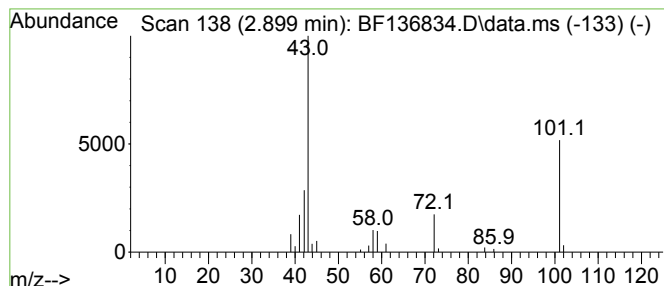
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.899	2.89 ng	57627	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	53
3		Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	42
4		Furazan-3-ol, 4-amino-	101	C2H3N3O2	159013-90-8	40
5		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	40



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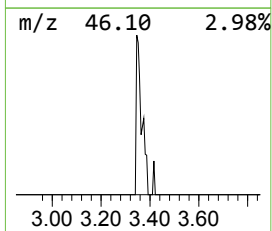
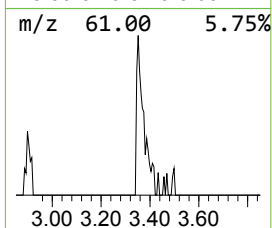
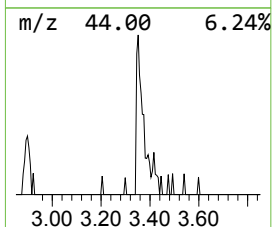
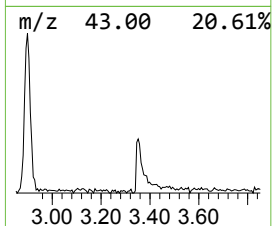
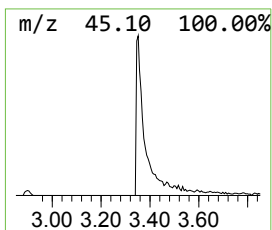
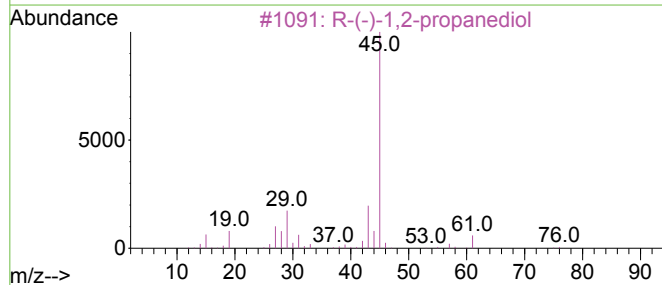
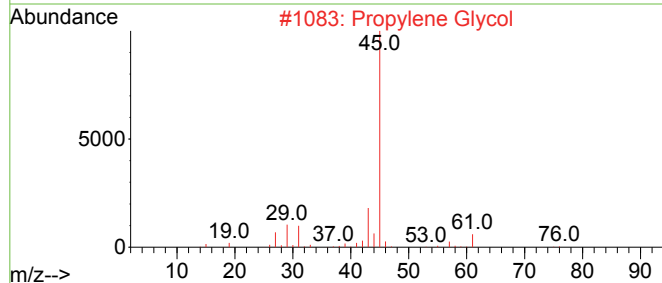
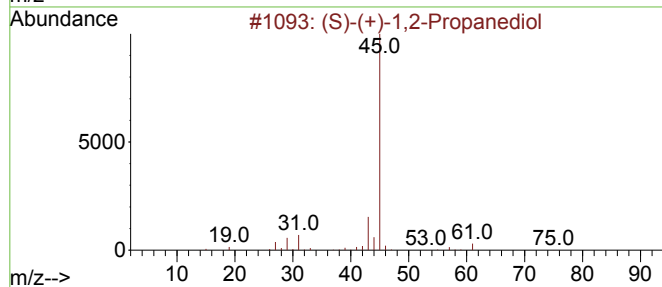
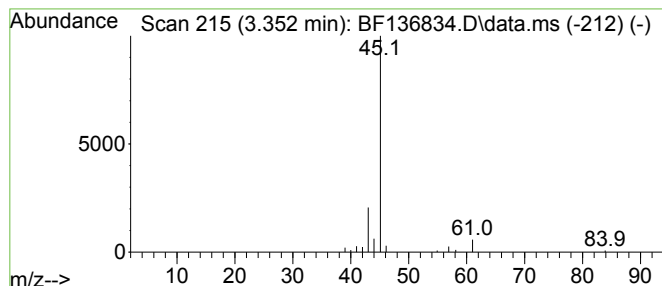
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.352	3.78 ng	75379	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2		Propylene Glycol	76	C3H8O2	000057-55-6	9
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4		Formamide	45	CH3NO	000075-12-7	5
5		Methoxyacetic acid, pentyl ester	160	C8H16O3	168920-35-2	4



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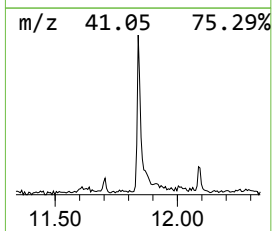
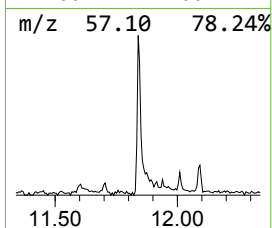
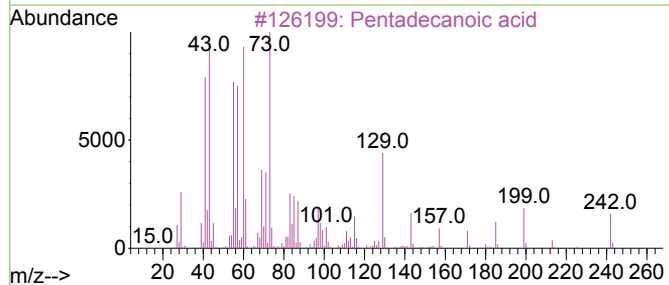
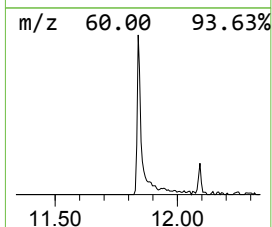
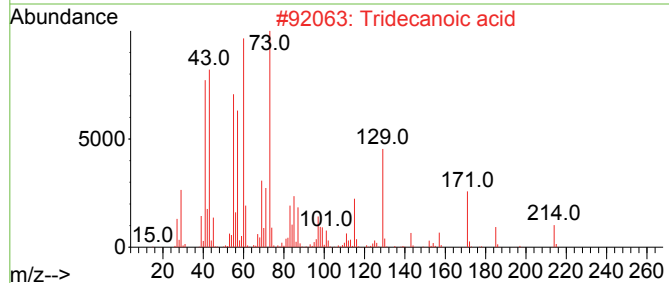
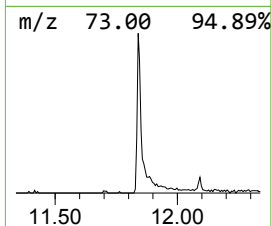
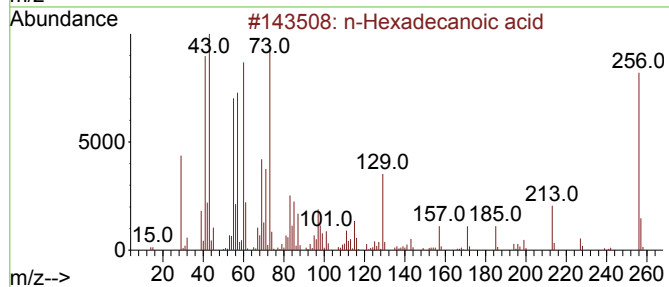
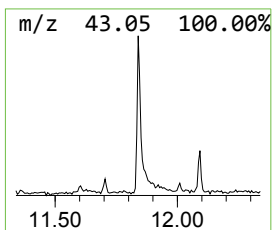
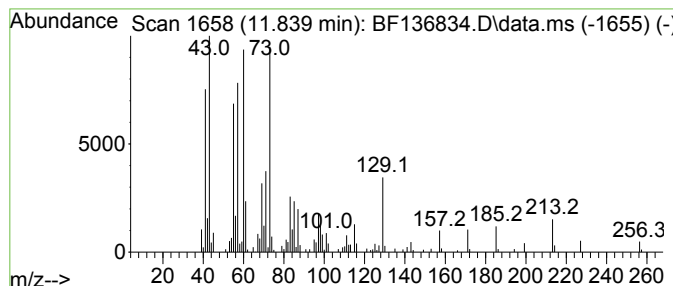
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	8.71 ng	263416	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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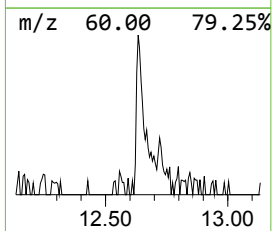
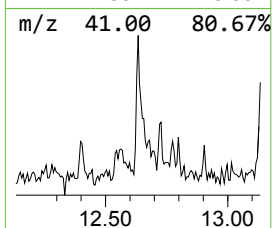
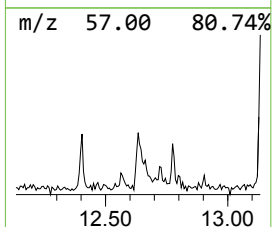
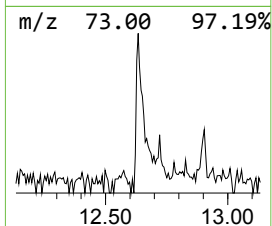
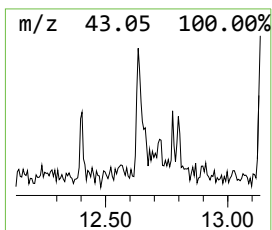
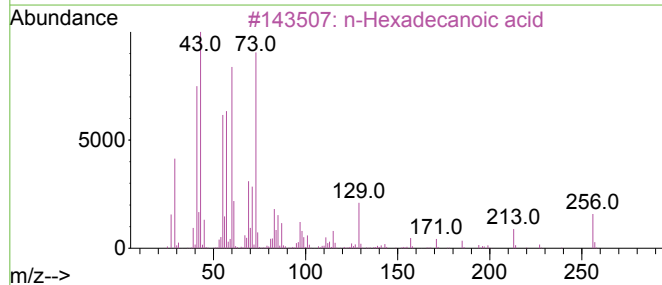
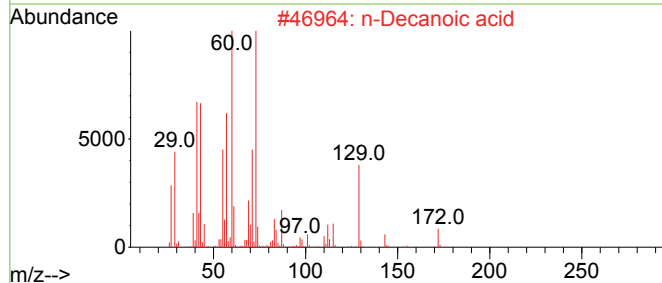
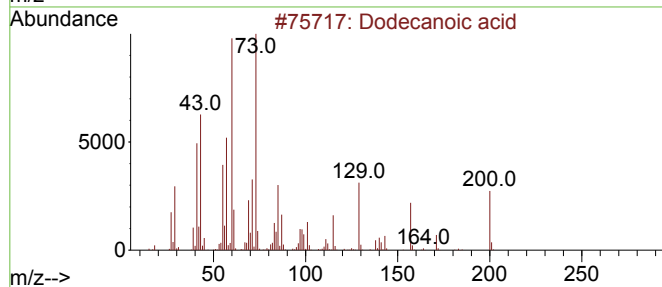
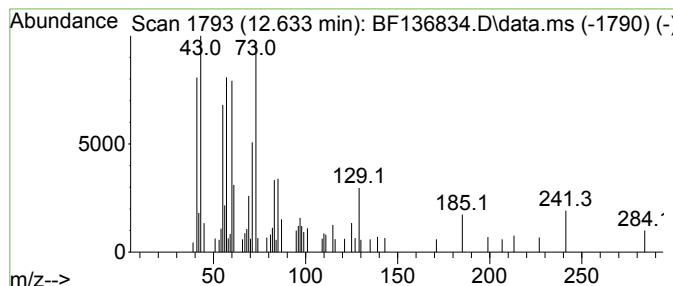
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	2.08 ng	62913	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	52
2			n-Decanoic acid	172	C10H20O2	000334-48-5	50
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
4			Octadecanoic acid	284	C18H36O2	000057-11-4	43
5			Lactose	342	C12H22O11	000063-42-3	43



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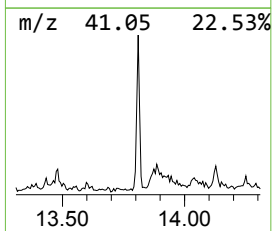
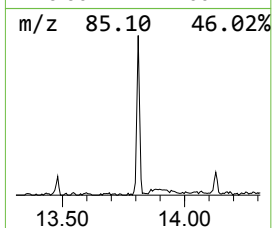
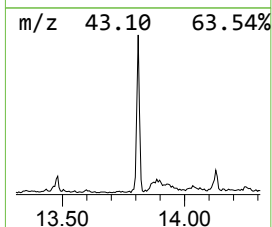
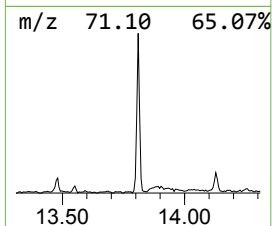
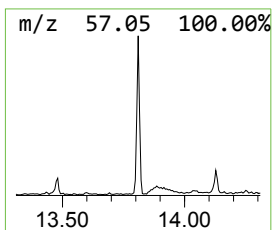
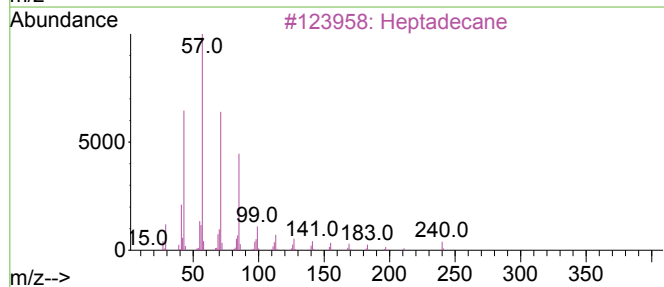
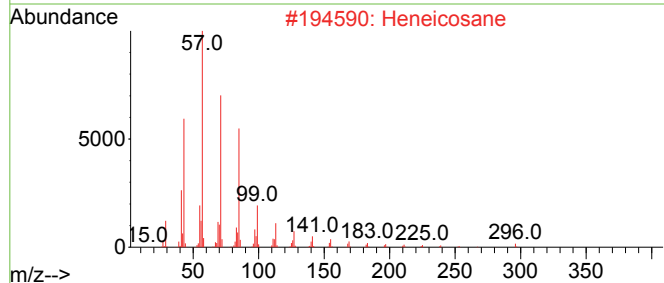
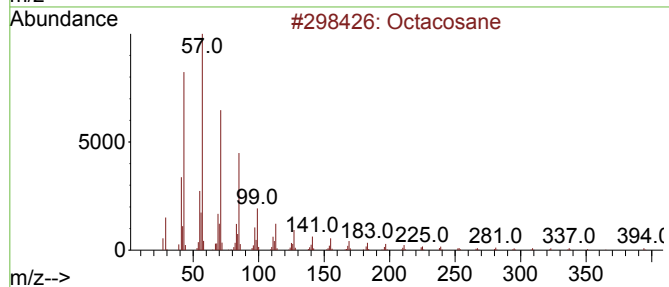
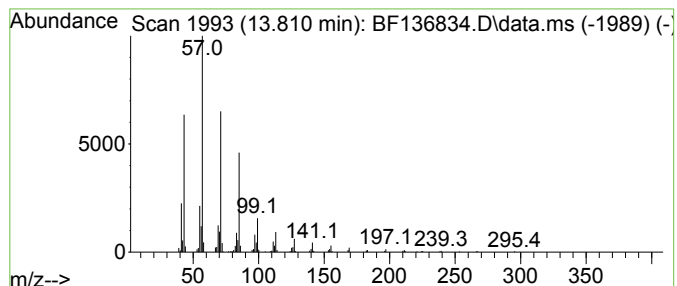
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	9.57 ng	192457	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Heptadecane	240	C17H36	000629-78-7	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136834.D
Acq On : 29 Dec 2023 17:44
Operator : CG\JU
Sample : 05897-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GHL-SS-36a

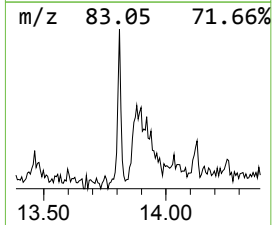
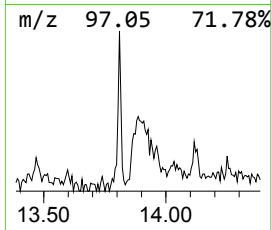
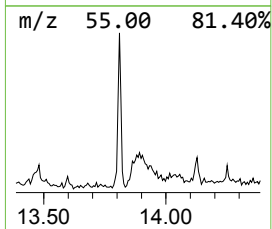
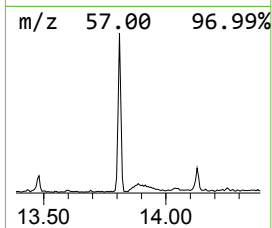
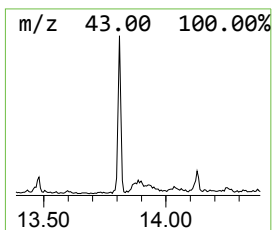
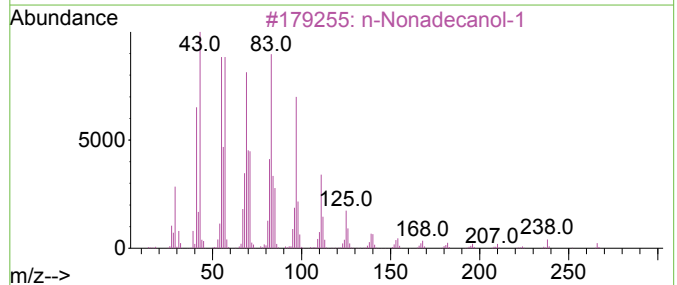
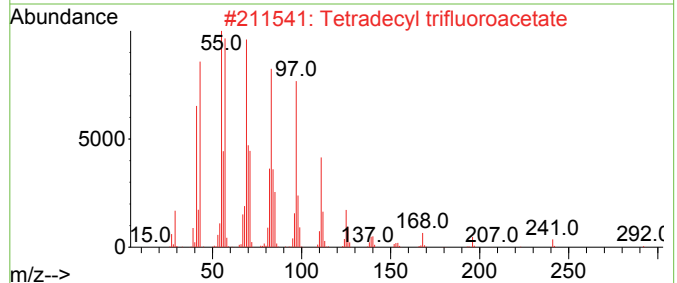
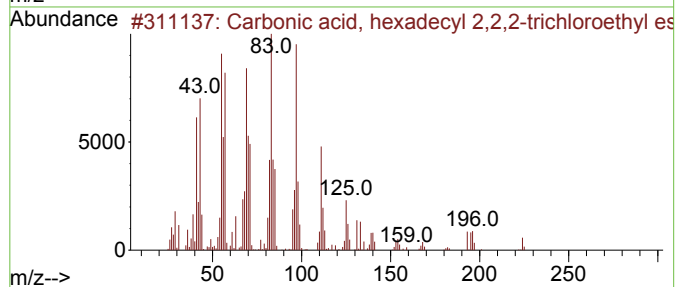
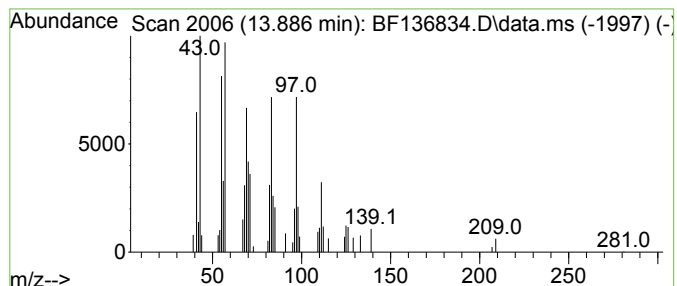
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Carbonic acid, hexadecyl 2,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	4.32 ng	86931	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	94
2			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	93
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	93
5			Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136834.D
Acq On : 29 Dec 2023 17:44
Operator : CG\JU
Sample : 05897-02
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ClientSampleId :
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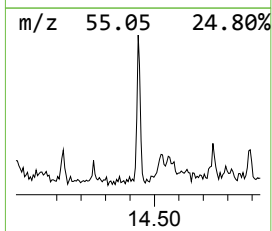
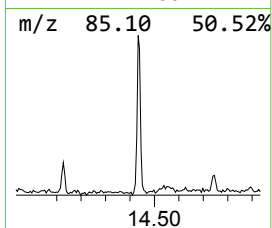
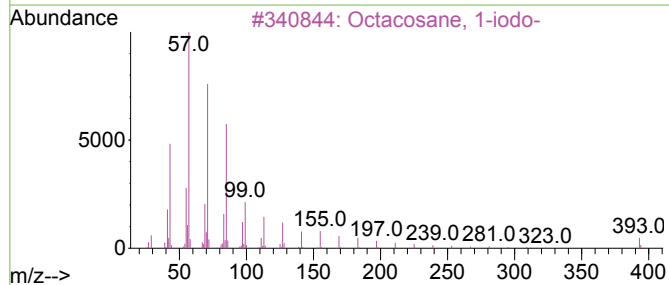
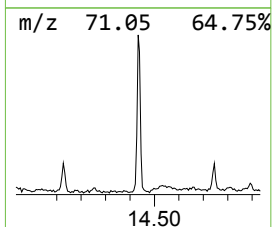
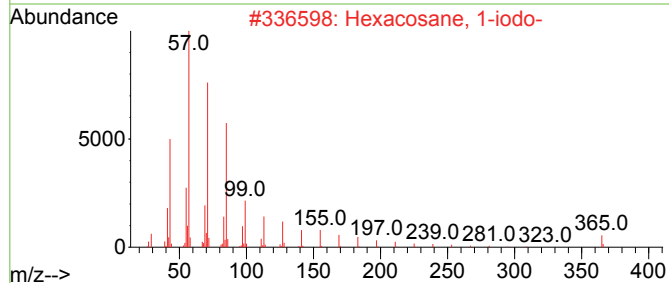
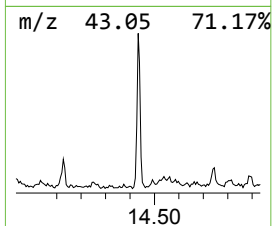
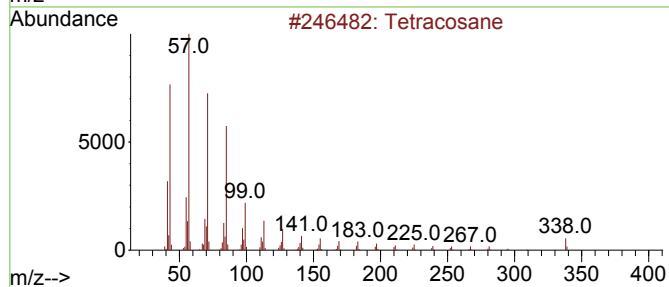
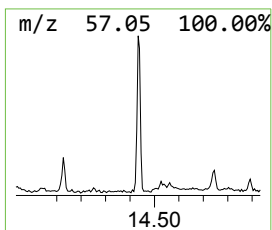
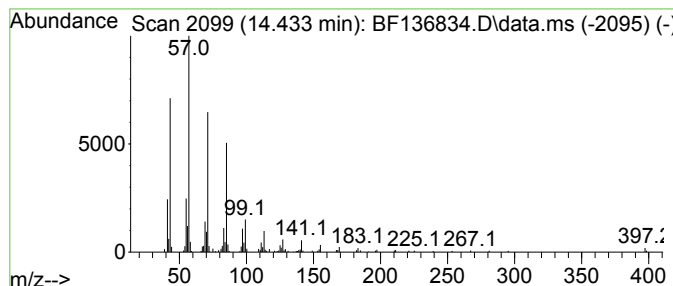
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	7.92 ng	159286	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91
3			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	91
4			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136834.D
Acq On : 29 Dec 2023 17:44
Operator : CG\JU
Sample : 05897-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

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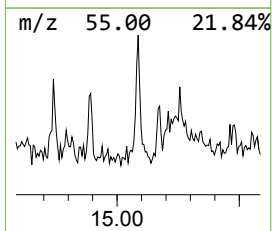
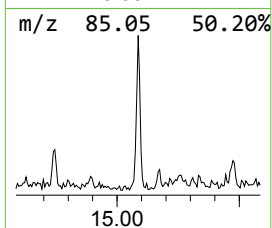
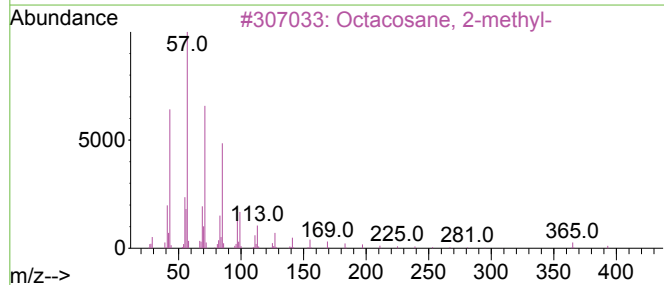
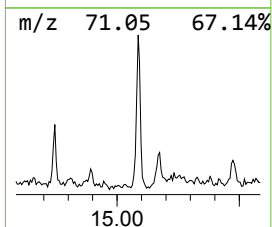
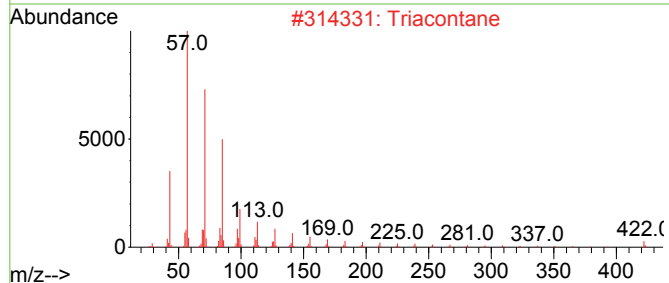
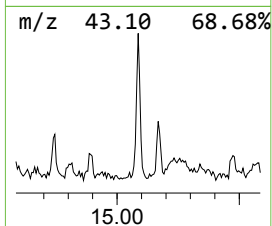
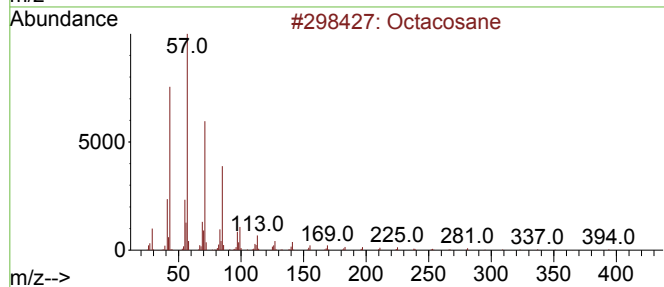
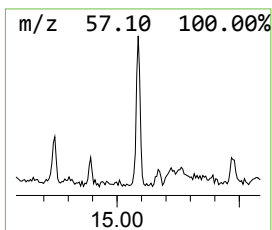
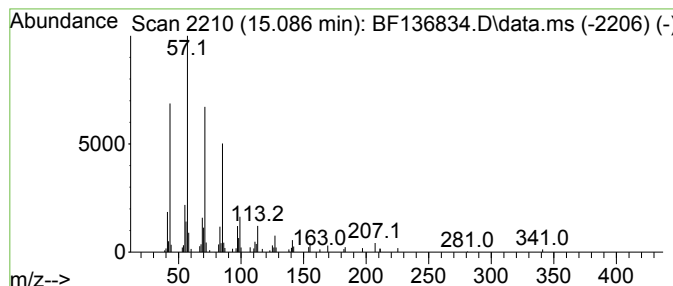
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	4.19 ng	79861	Perylene-d12	15.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136834.D
Acq On : 29 Dec 2023 17:44
Operator : CG\JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

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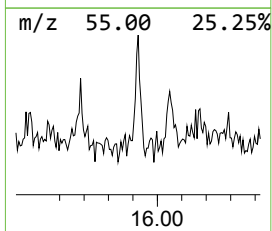
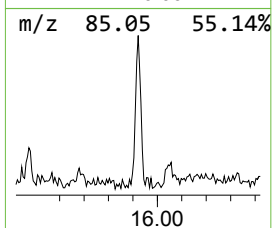
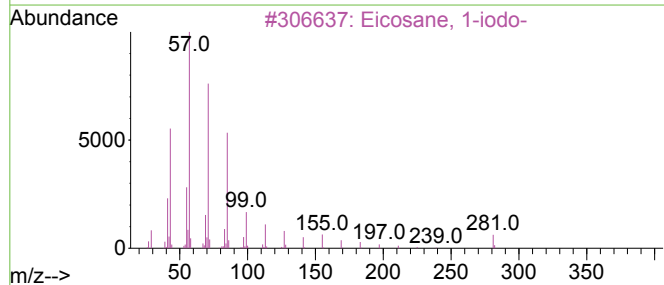
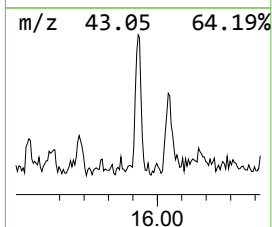
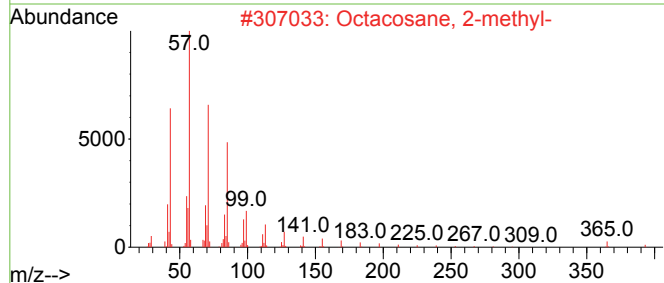
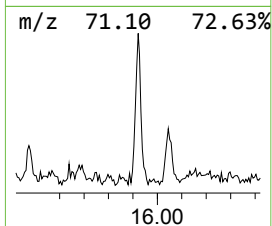
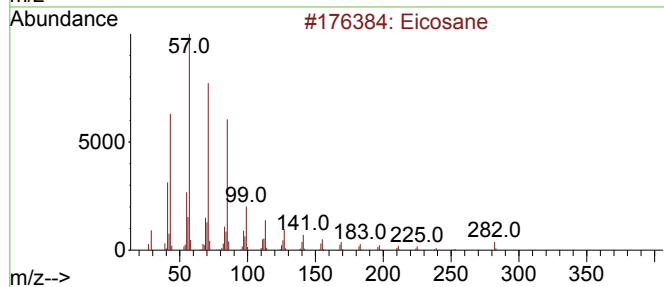
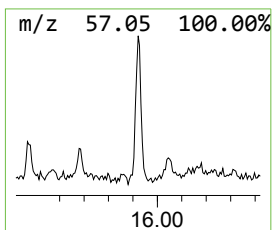
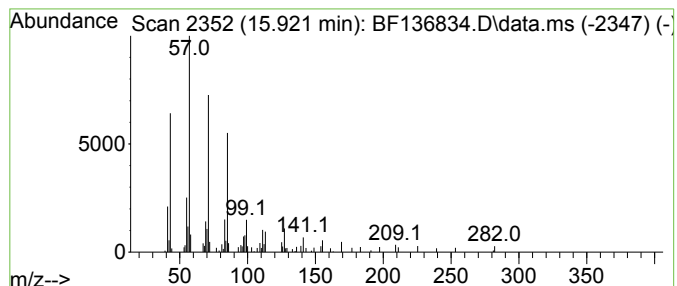
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	3.93 ng	74815	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90
4			Docosane	310	C22H46	000629-97-0	87
5			Triacontane	422	C30H62	000638-68-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136834.D
Acq On : 29 Dec 2023 17:44
Operator : CG\JU
Sample : 05897-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

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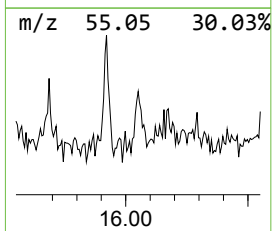
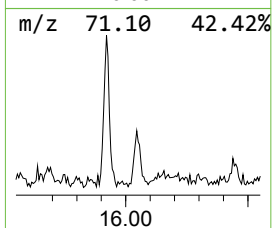
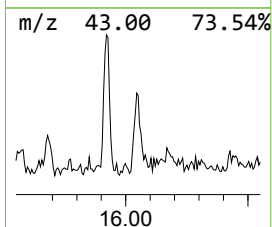
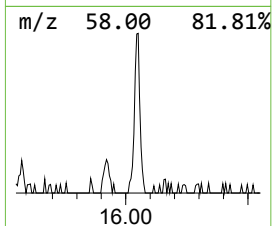
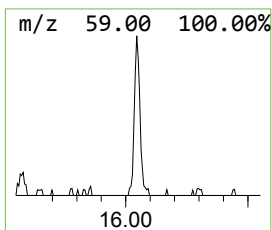
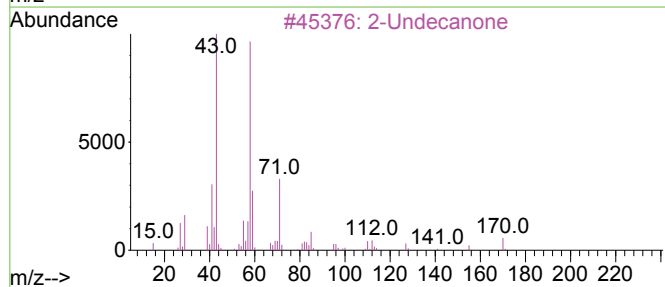
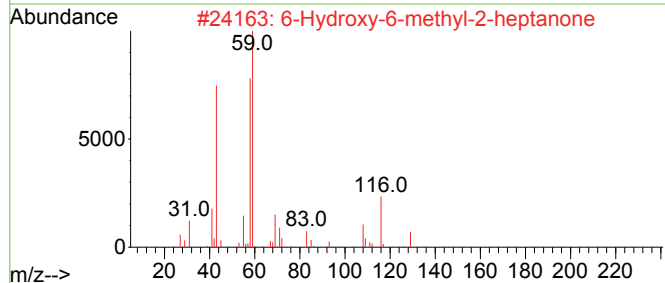
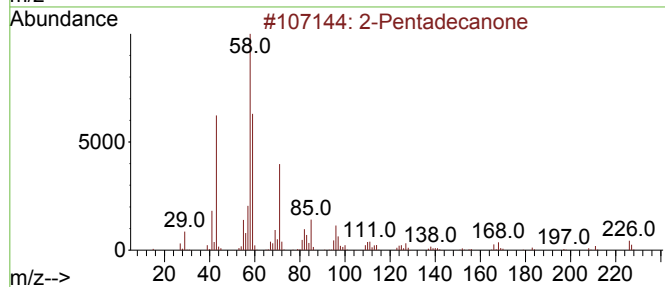
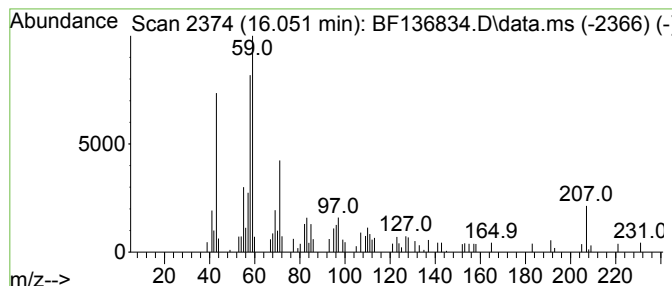
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Pentadecanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.051	4.19 ng	79860	Perylene-d12	15.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentadecanone	226	C15H30O	002345-28-0	53
2		6-Hydroxy-6-methyl-2-heptanone	144	C8H16O2	1000432-37-3	43
3		2-Undecanone	170	C11H22O	000112-12-9	43
4		2-Dodecanone	184	C12H24O	006175-49-1	43
5		Oxirane, tetramethyl-	100	C6H12O	005076-20-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136834.D
Acq On : 29 Dec 2023 17:44
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Misc :
ALS Vial : 18 Sample Multiplier: 1

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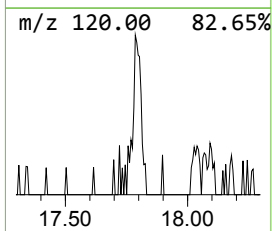
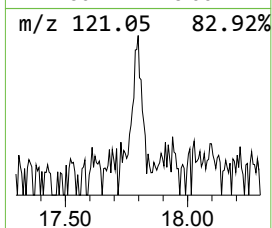
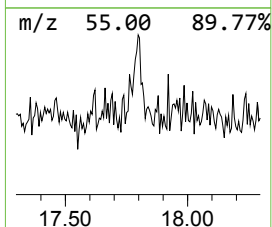
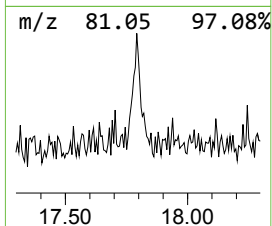
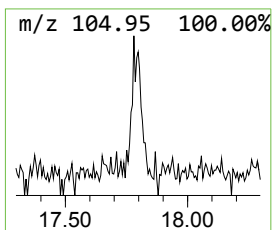
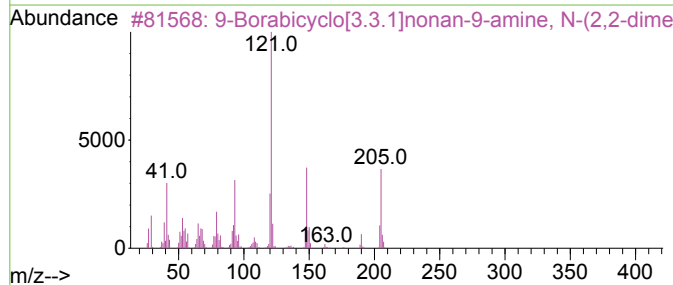
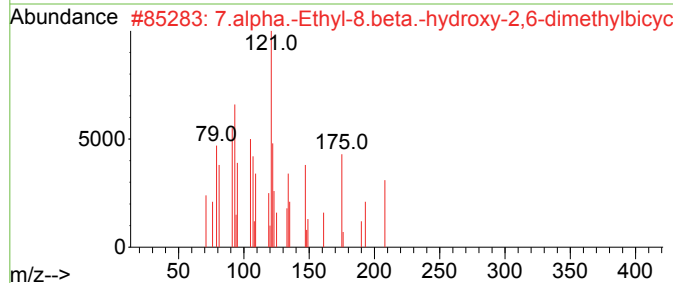
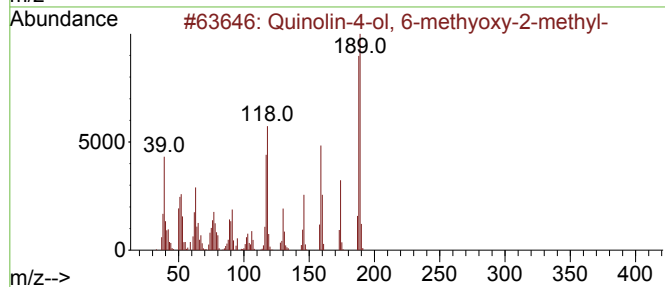
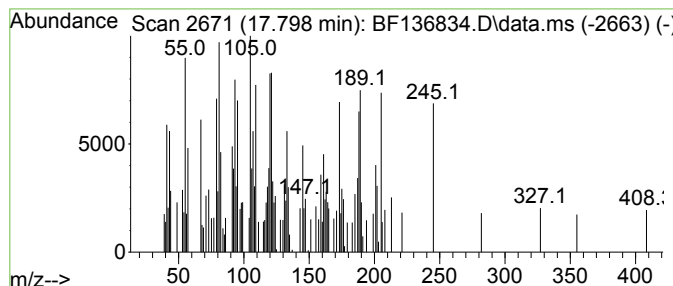
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.798 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.798	5.19 ng	98783	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Quinolin-4-ol, 6-methoxy-2-methyl-	189	C11H11NO2	015644-90-3	25
2			7.alpha.-Ethyl-8.beta.-hydroxy-2...	208	C14H24O	1000077-92-4	25
3			9-Borabicyclo[3.3.1]nonan-9-amin...	205	C13H24BN	143122-94-5	18
4			5.alpha.-Hydroxy-4.alpha.,8,10,1...	220	C15H24O	141922-47-6	18
5			(R)-2-((4aS,8aR)-4a-Methyl-8-met...	220	C15H24O	028102-68-3	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136834.D
Acq On : 29 Dec 2023 17:44
Operator : CG\JU
Sample : 05897-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-36a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
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(S)-(+)-1,2-Pro...	3.352	3.8	ng	75379	1	6.781	398313	20.0
n-Hexadecanoic ...	11.839	8.7	ng	263416	4	11.304	605050	20.0
Dodecanoic acid	12.633	2.1	ng	62913	4	11.304	605050	20.0
Octacosane	13.810	9.6	ng	192457	5	13.963	402173	20.0
Carbonic acid, ...	13.886	4.3	ng	86931	5	13.963	402173	20.0
Tetracosane	14.433	7.9	ng	159286	5	13.963	402173	20.0
triacontane	15.086	4.2	ng	79861	6	15.445	380861	20.0
Eicosane	15.921	3.9	ng	74815	6	15.445	380861	20.0
2-Pentadecanone	16.051	4.2	ng	79860	6	15.445	380861	20.0
unknown17.798	17.798	5.2	ng	98783	6	15.445	380861	20.0