

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
 Data File : BF126262.D
 Acq On : 18 Dec 2021 19:20
 Operator : JU/CG
 Sample : M5079-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 338

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126262.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	15	rVB	886632	1110536	19.65%	2.285%
2	2.240	18	26	34	rVB	96870	127253	2.25%	0.262%
3	3.393	199	222	225	rBV	636187	2964221	52.46%	6.098%
4	5.034	492	501	509	rBV	623463	895789	15.85%	1.843%
5	5.434	563	569	572	rBV	4800292	5240267	92.74%	10.781%
6	5.828	633	636	640	rVB	98258	87884	1.56%	0.181%
7	6.446	735	741	745	rBV	4441730	5650508	100.00%	11.625%
8	6.816	800	804	807	rBV	1653631	1385578	24.52%	2.851%
9	7.375	893	899	902	rBV	3344892	3685502	65.22%	7.582%
10	7.457	910	913	923	rVB	56678	71963	1.27%	0.148%
11	8.004	1002	1006	1017	rBV	561257	644292	11.40%	1.325%
12	8.098	1017	1022	1025	rBV	2100402	1984443	35.12%	4.083%
13	9.175	1200	1205	1208	rBV	4910295	5175884	91.60%	10.648%
14	9.263	1216	1220	1224	rBV2	72489	85147	1.51%	0.175%
15	9.316	1224	1229	1243	rVB	254104	475357	8.41%	0.978%
16	9.669	1286	1289	1294	rBV2	94116	158561	2.81%	0.326%
17	9.851	1312	1320	1324	rBV	2481162	2193774	38.82%	4.513%
18	10.263	1387	1390	1393	rBV2	163466	158116	2.80%	0.325%
19	10.563	1437	1441	1444	rBV	65381	61574	1.09%	0.127%
20	10.639	1449	1454	1457	rBV	2724885	2517235	44.55%	5.179%
21	10.857	1487	1491	1499	rVB2	56277	85416	1.51%	0.176%
22	11.210	1549	1551	1560	rVB3	78272	119672	2.12%	0.246%
23	11.298	1563	1566	1569	rBV	219154	197992	3.50%	0.407%
24	11.333	1569	1572	1575	rVV	2226721	2056829	36.40%	4.232%
25	11.404	1579	1584	1587	rBV6	95877	124268	2.20%	0.256%
26	11.504	1598	1601	1608	rVB	144267	150223	2.66%	0.309%
27	11.639	1621	1624	1630	rVB5	40685	61015	1.08%	0.126%
28	11.733	1637	1640	1645	rVB	100171	99547	1.76%	0.205%
29	11.863	1660	1662	1665	rVB2	85236	70194	1.24%	0.144%
30	11.904	1665	1669	1672	rVB	181949	171613	3.04%	0.353%
31	11.945	1672	1676	1679	rBV4	42044	60950	1.08%	0.125%
32	12.122	1704	1706	1709	rBV3	70976	64959	1.15%	0.134%
33	12.322	1737	1740	1745	rBV2	66815	79317	1.40%	0.163%
34	12.380	1746	1750	1754	rVV2	74302	87650	1.55%	0.180%
35	12.545	1775	1778	1780	rBV	189322	157461	2.79%	0.324%
36	12.769	1811	1816	1821	rVB	184011	204576	3.62%	0.421%

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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-BF121521.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.927	1838	1843	1846	rBV	4418398	4520024	79.99%	9.299%
38	13.839	1990	1998	2012	rBV	403546	868813	15.38%	1.787%
39	13.969	2015	2020	2023	rBV	1518694	1457372	25.79%	2.998%
40	14.069	2031	2037	2043	rBV	432296	527854	9.34%	1.086%
41	14.480	2104	2107	2114	rVB8	43457	79274	1.40%	0.163%
42	14.833	2163	2167	2173	rVB	407883	406711	7.20%	0.837%
43	14.992	2191	2194	2197	rBV	61105	85791	1.52%	0.176%
44	15.092	2208	2211	2215	rVB2	93487	97518	1.73%	0.201%
45	15.145	2215	2220	2222	rBV6	40981	72233	1.28%	0.149%
46	15.292	2242	2245	2251	rVB	52418	66478	1.18%	0.137%
47	15.351	2251	2255	2260	rBV	64105	79124	1.40%	0.163%
48	15.416	2261	2266	2271	rBV	972545	1185692	20.98%	2.439%
49	15.468	2271	2275	2278	rVB	76438	102622	1.82%	0.211%
50	15.898	2343	2348	2354	rVB	94003	134907	2.39%	0.278%
51	15.980	2356	2362	2378	rVV10	46412	181910	3.22%	0.374%
52	16.392	2427	2432	2439	rVB3	61888	110839	1.96%	0.228%
53	16.980	2526	2532	2540	rBV4	44342	95907	1.70%	0.197%
54	17.668	2644	2649	2657	rVB4	32723	68855	1.22%	0.142%

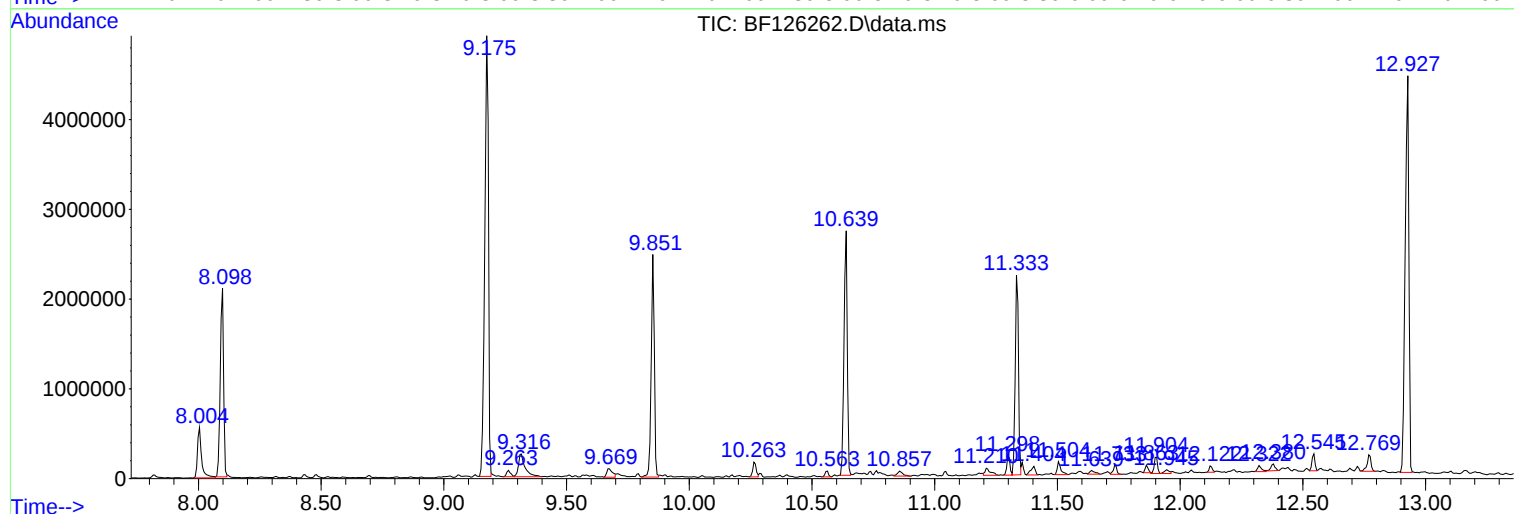
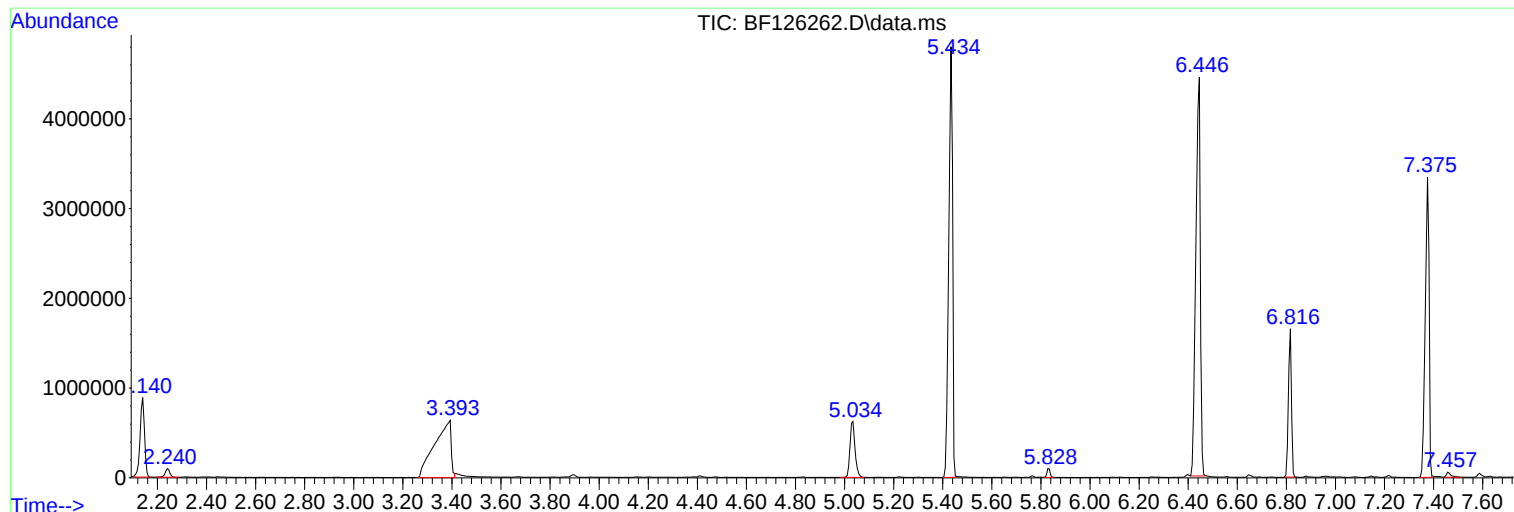
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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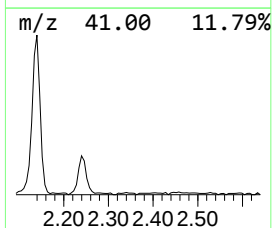
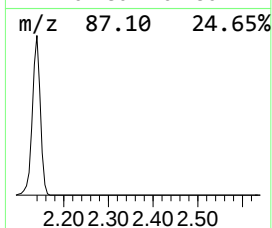
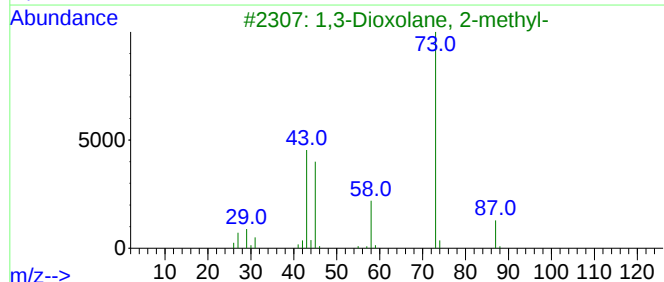
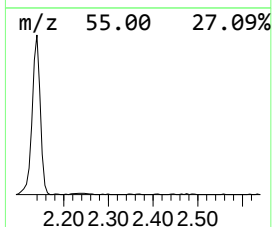
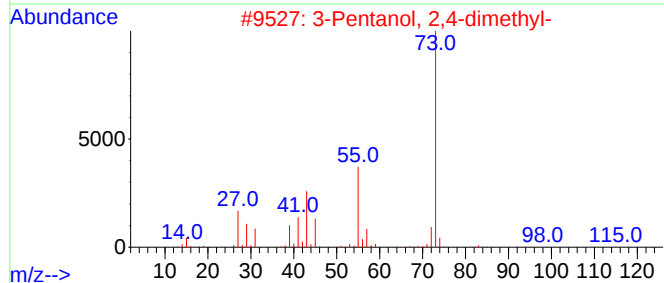
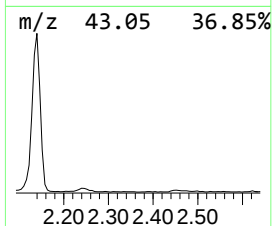
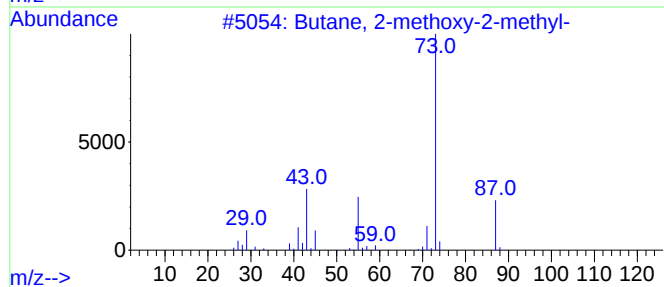
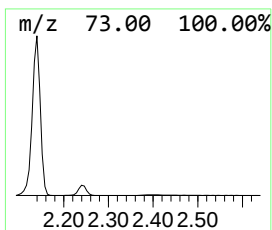
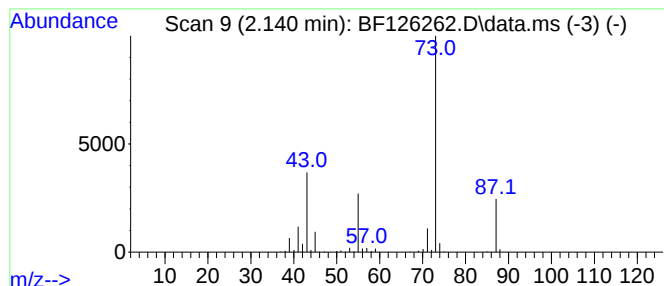
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	16.03 ng	1110540	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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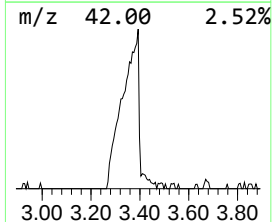
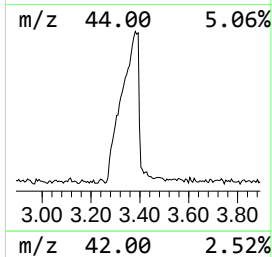
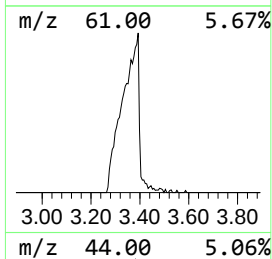
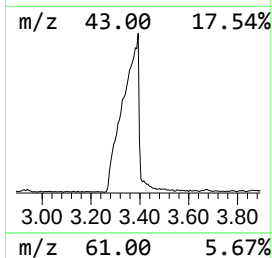
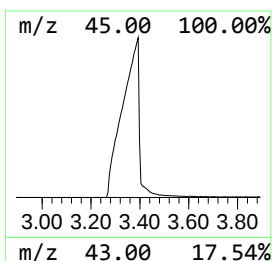
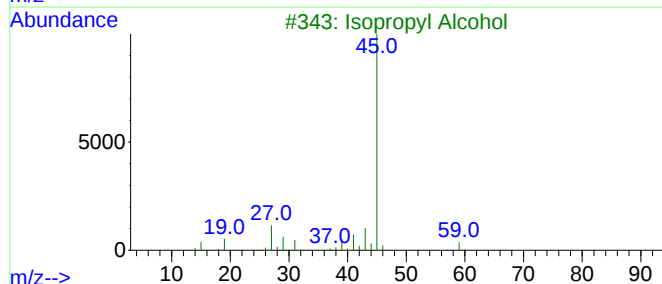
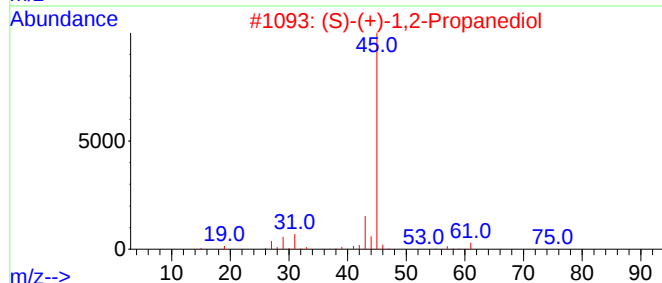
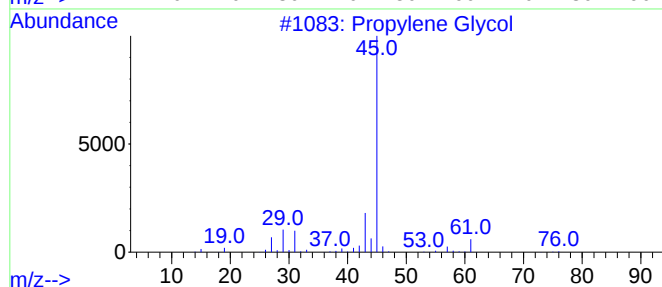
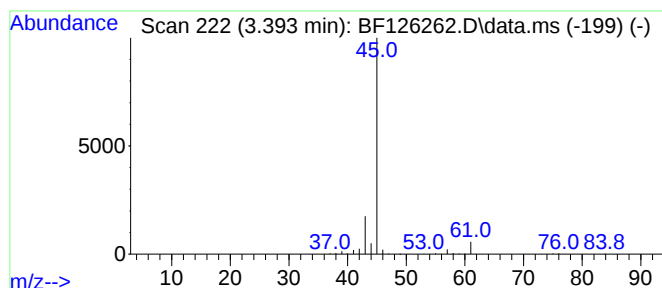
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	42.79 ng	2964220	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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ALS Vial : 16 Sample Multiplier: 1

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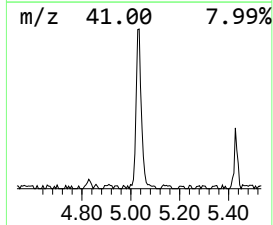
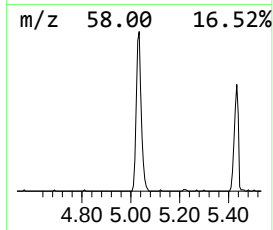
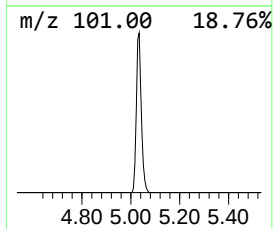
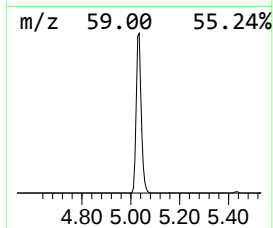
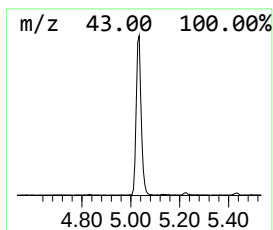
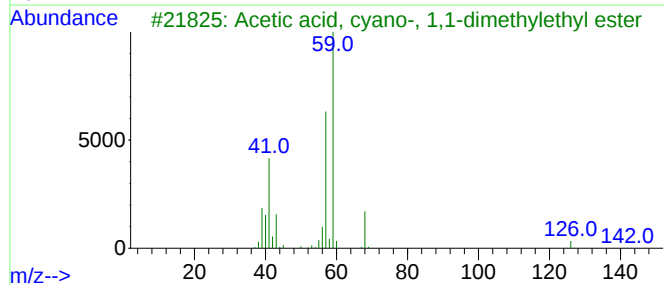
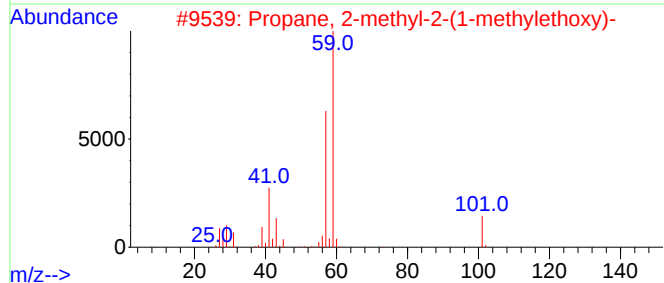
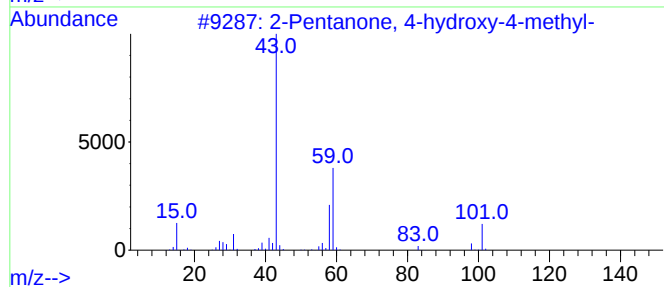
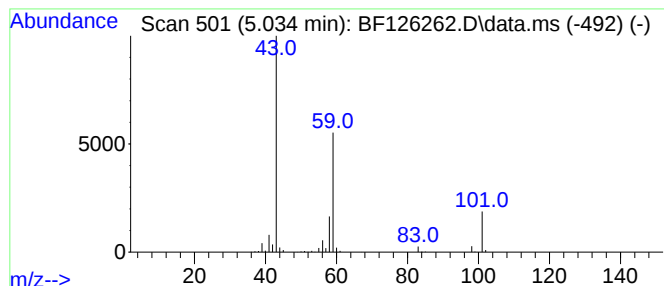
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	12.93 ng	895789	1,4-Dichlorobenzene-d4	6.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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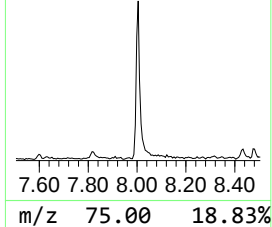
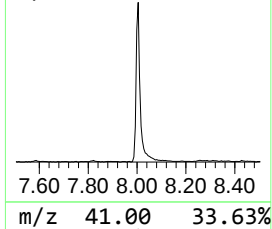
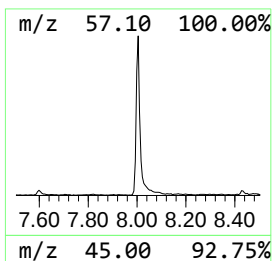
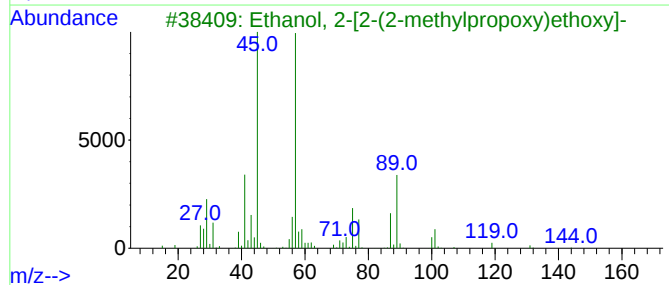
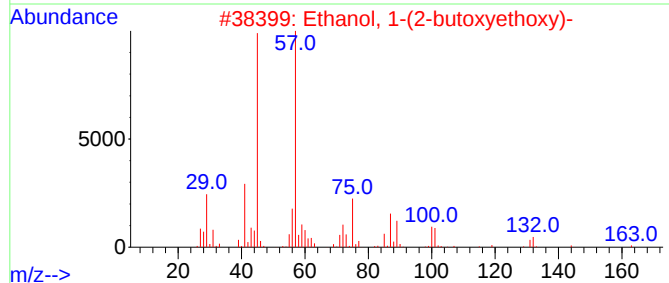
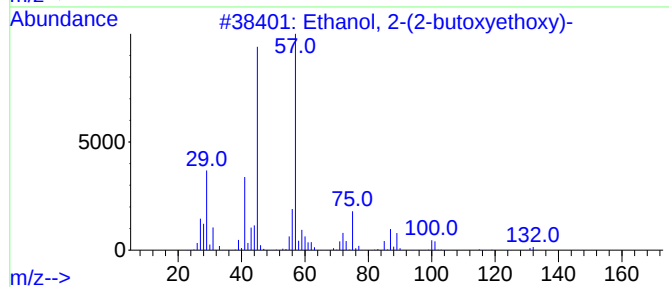
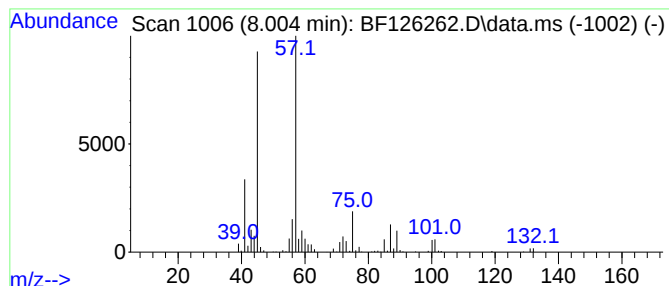
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	6.49 ng	644292	Naphthalene-d8	8.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	50



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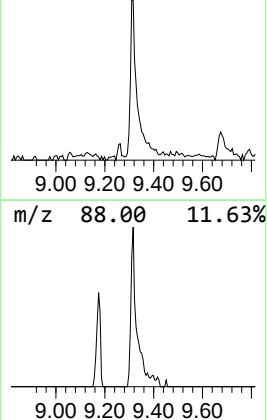
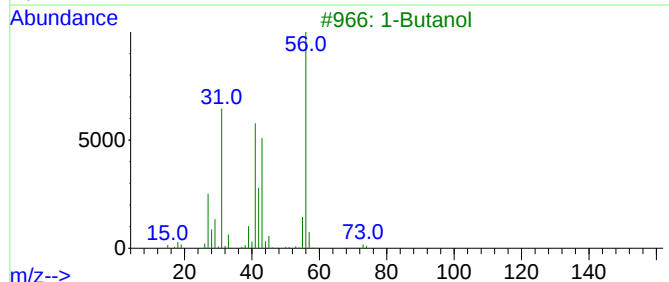
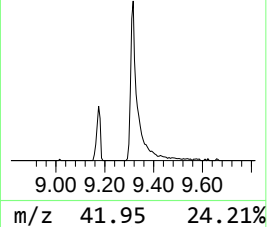
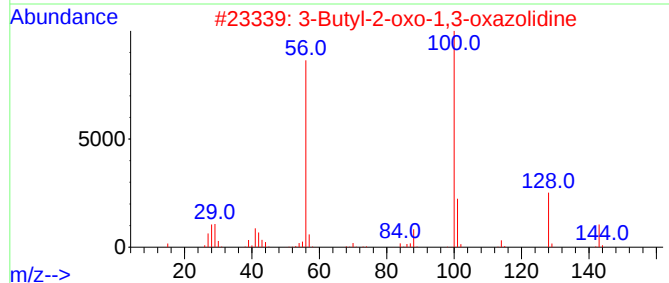
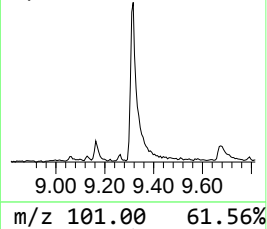
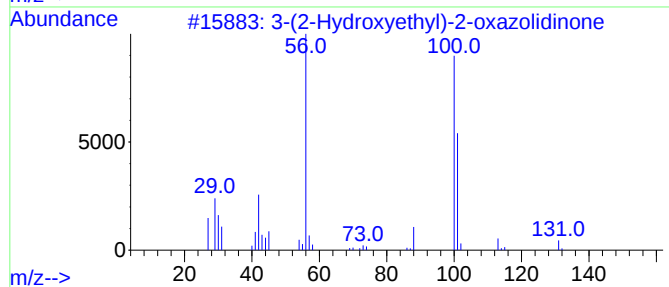
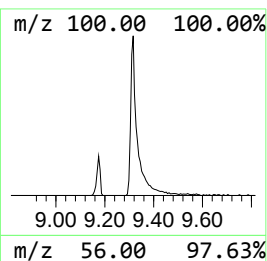
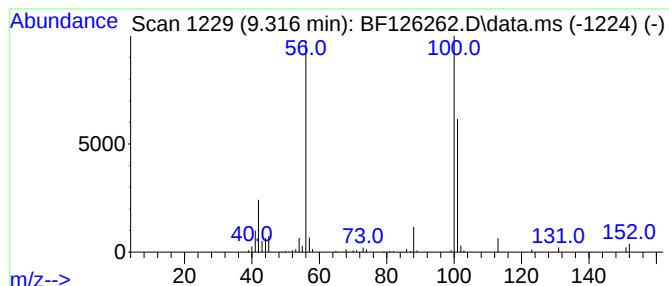
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.316	4.33 ng	475357	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	87
2			3-Butyl-2-oxo-1,3-oxazolidine	143	C7H13NO2	023288-01-9	38
3			1-Butanol	74	C4H10O	000071-36-3	27
4			Methanamine, N-(1-methylbutylidene...	99	C6H13N	022431-09-0	27
5			N-(3-Hydroxypropyl)morpholine	145	C7H15NO2	1000425-83-2	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126262.D
Acq On : 18 Dec 2021 19:20
Operator : JU/CG
Sample : M5079-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

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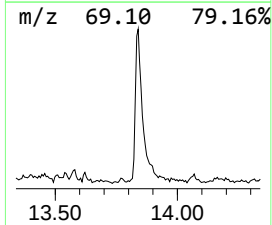
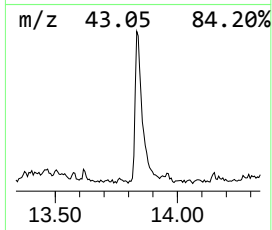
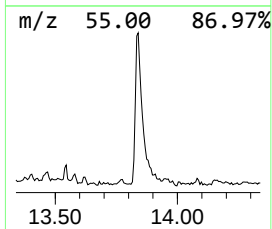
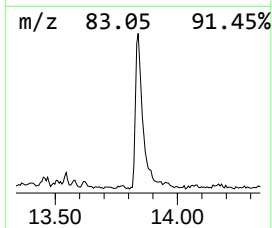
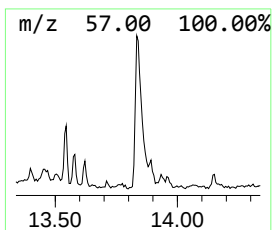
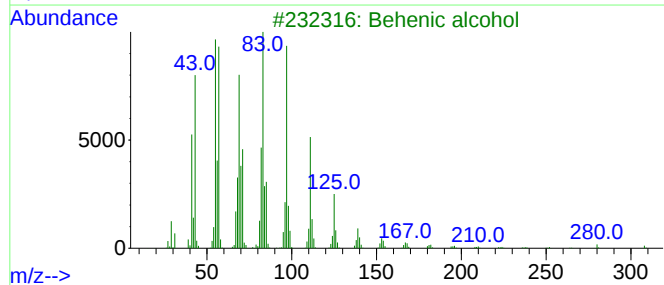
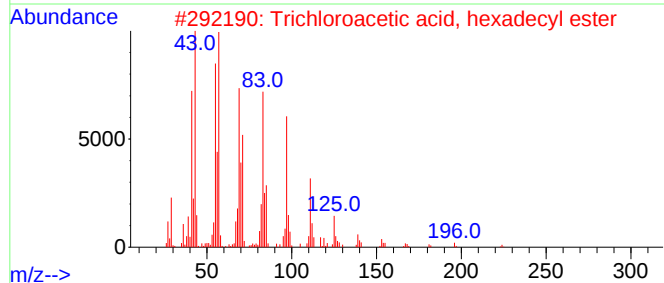
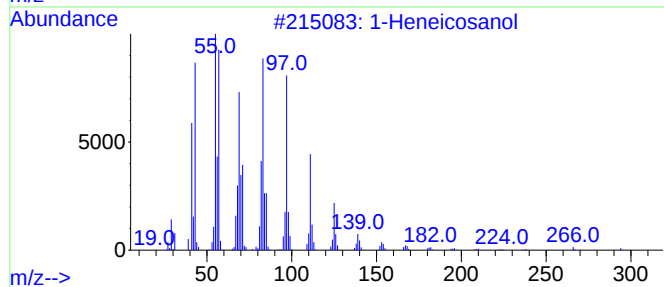
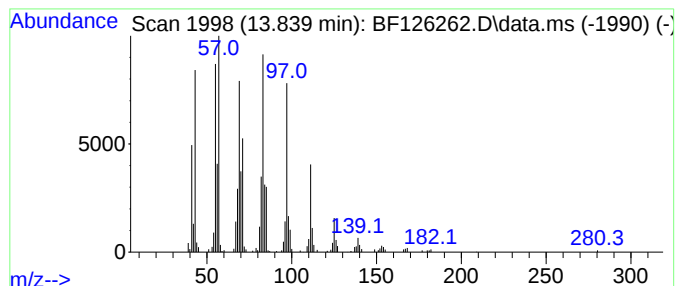
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	11.92 ng	868813	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			Behenic alcohol	326	C22H46O	000661-19-8	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126262.D
Acq On : 18 Dec 2021 19:20
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Sample : M5079-04
Misc :
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Instrument :
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ClientSampleId :
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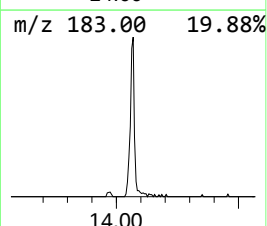
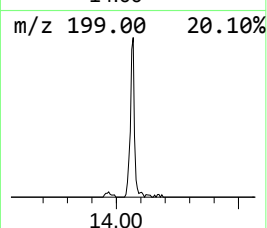
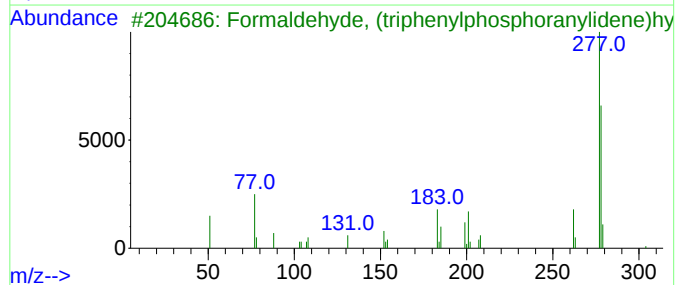
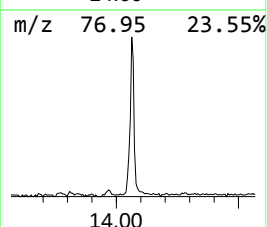
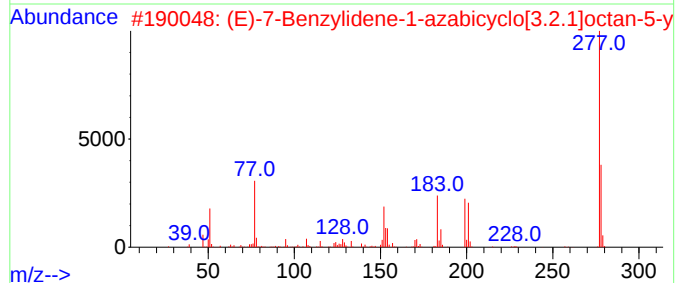
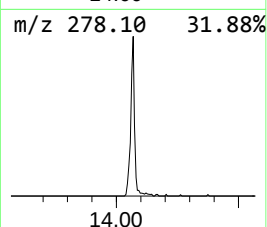
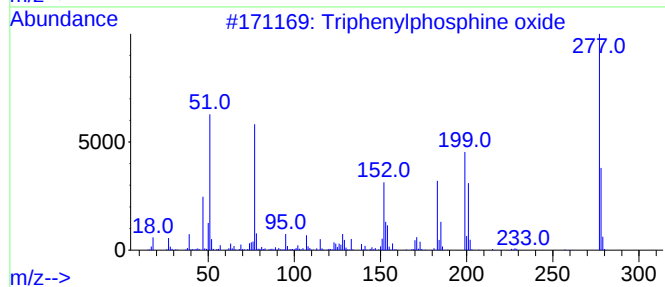
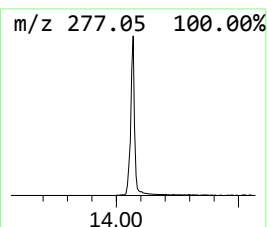
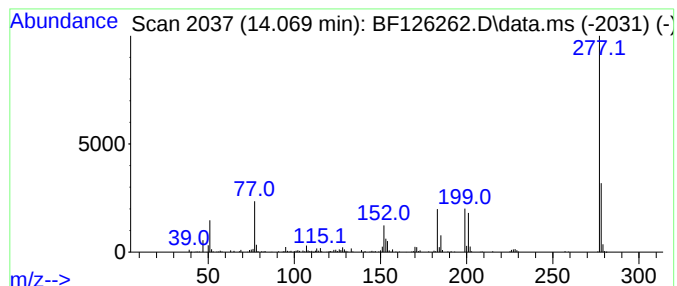
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.069	7.24 ng	527854	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	43
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126262.D
Acq On : 18 Dec 2021 19:20
Operator : JU/CG
Sample : M5079-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

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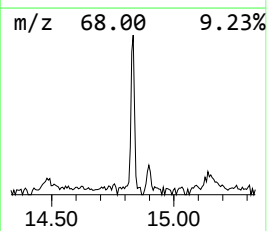
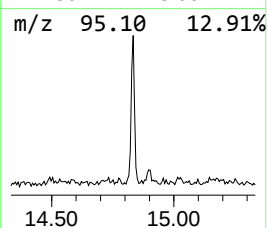
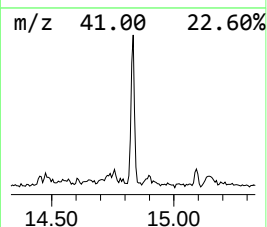
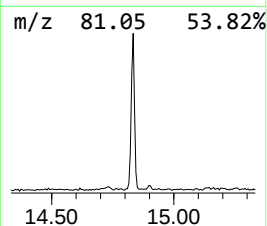
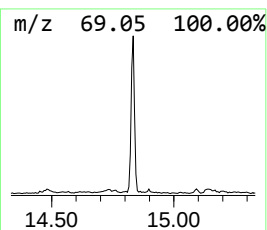
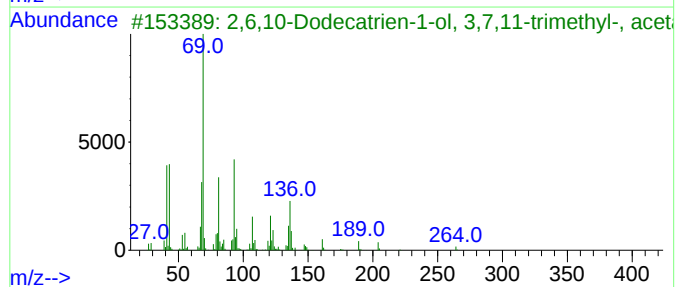
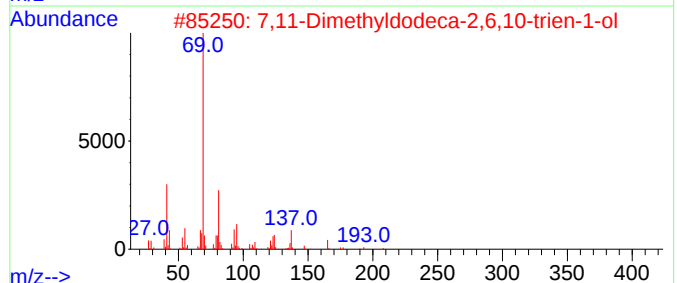
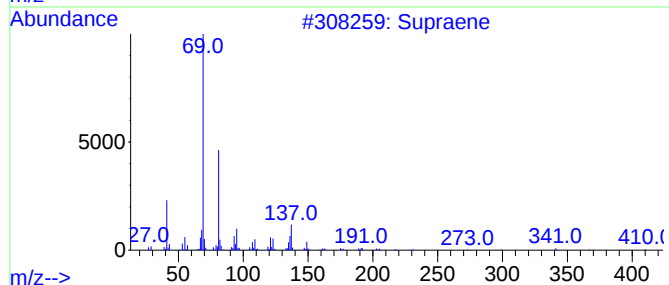
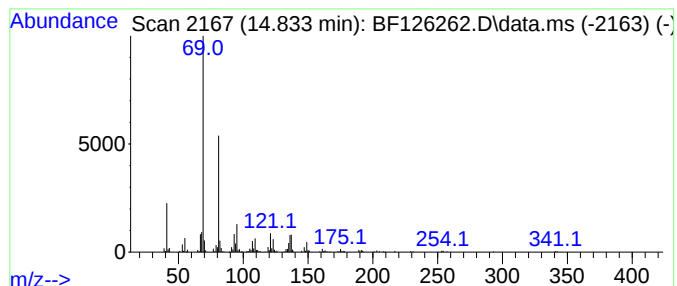
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	6.86 ng	406711	Perylene-d12	15.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
3			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
4			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	53
5			2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126262.D
Acq On : 18 Dec 2021 19:20
Operator : JU/CG
Sample : M5079-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

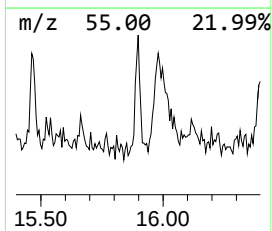
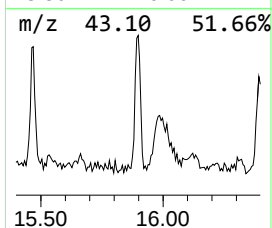
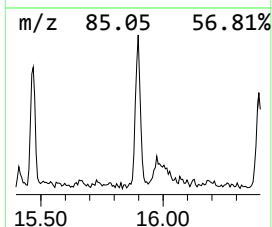
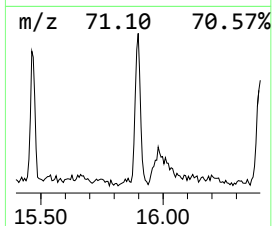
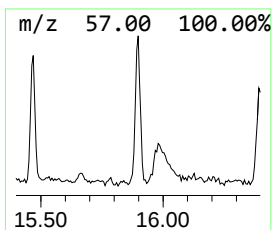
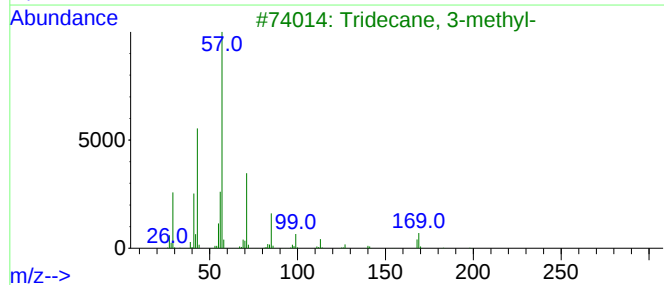
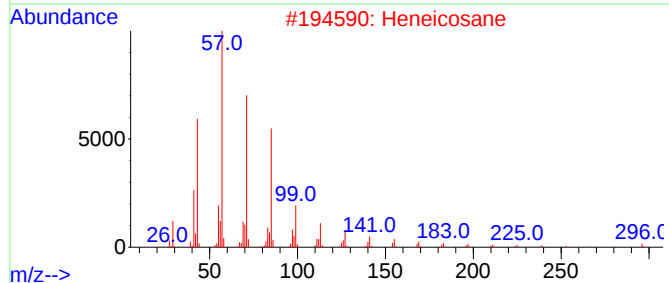
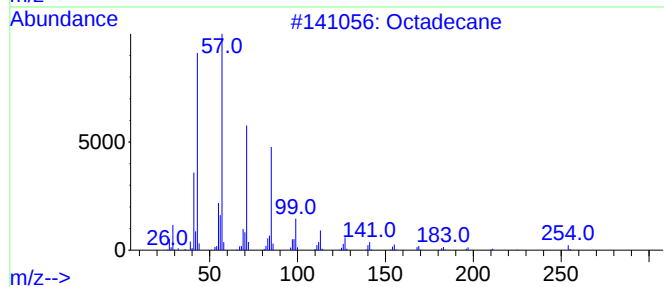
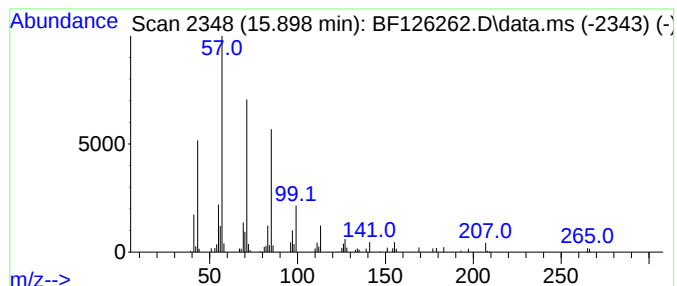
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.898	2.28 ng	134907	Perylene-d12	15.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	86
2	Heneicosane	296	C21H44	000629-94-7	83
3	Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126262.D
Acq On : 18 Dec 2021 19:20
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Sample : M5079-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

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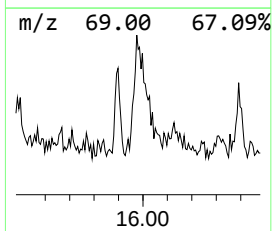
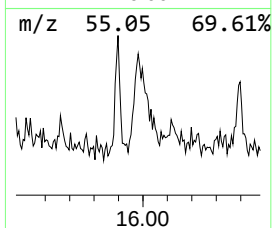
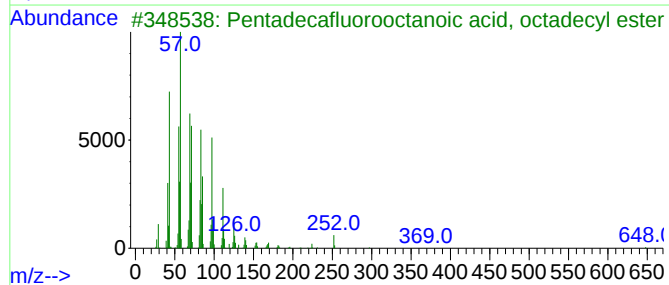
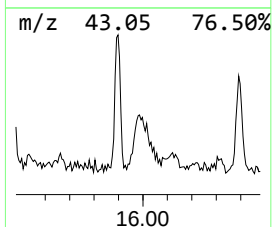
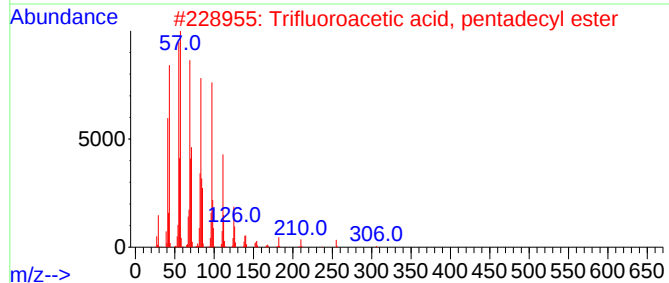
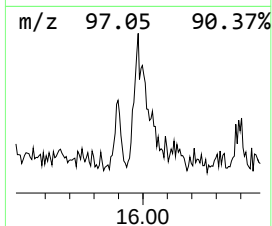
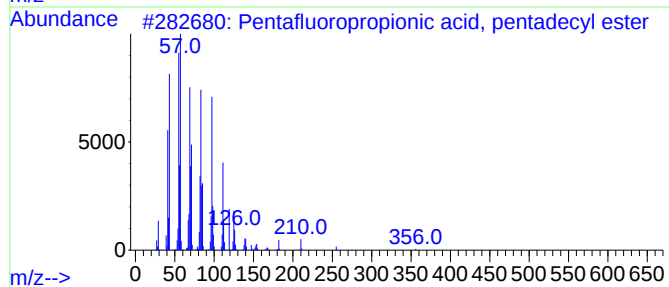
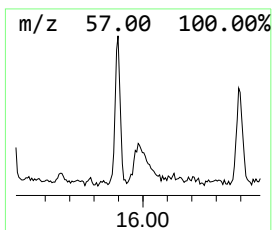
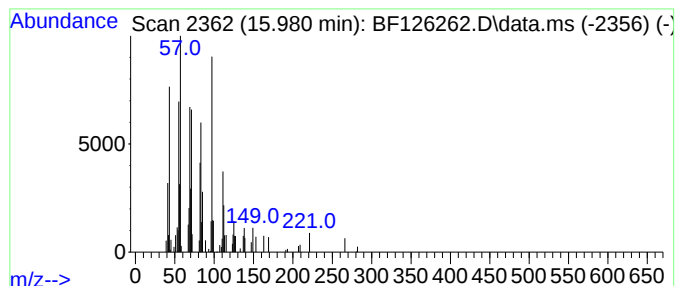
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.980	3.07 ng	181910	Perylene-d12	15.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	60
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	60
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	60
4			Propyl triacontyl ether	481	C33H68O	1000406-28-6	58
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126262.D
Acq On : 18 Dec 2021 19:20
Operator : JU/CG
Sample : M5079-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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
Butane, 2-metho...	2.140	16.0	ng	1110540	1	6.816	1385580	20.0
Propylene Glycol	3.393	42.8	ng	2964220	1	6.816	1385580	20.0
2-Pentanone, 4-...	5.034	12.9	ng	895789	1	6.816	1385580	20.0
Ethanol, 2-(2-b...	8.004	6.5	ng	644292	2	8.098	1984440	20.0
3-(2-Hydroxyeth...	9.316	4.3	ng	475357	3	9.851	2193770	20.0
1-Heneicosanol	13.839	11.9	ng	868813	5	13.969	1457370	20.0
Triphenylphosph...	14.069	7.2	ng	527854	5	13.969	1457370	20.0
Supraene	14.833	6.9	ng	406711	6	15.416	1185690	20.0
Octadecane	15.898	2.3	ng	134907	6	15.416	1185690	20.0
Pentafluoroprop...	15.980	3.1	ng	181910	6	15.416	1185690	20.0