

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
 Data File : BF126926.D
 Acq On : 17 Feb 2022 14:52
 Operator : CG\JU
 Sample : N1564-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126926.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.499	201	206	221	rBV	73567	143816	3.93%	0.556%
2	5.175	484	491	498	rVB	33540	44760	1.22%	0.173%
3	5.551	550	555	558	rBV	3020872	2916360	79.66%	11.278%
4	6.551	719	725	728	rBV	2892629	3096727	84.59%	11.975%
5	6.928	785	789	792	rBV	946012	722817	19.74%	2.795%
6	7.493	879	885	888	rBV	2232767	2101961	57.42%	8.129%
7	8.104	985	989	1000	rBV	179187	153633	4.20%	0.594%
8	8.210	1003	1007	1010	rBV	1213983	988432	27.00%	3.822%
9	9.287	1184	1190	1193	rBV	4302120	3660991	100.00%	14.157%
10	9.763	1268	1271	1280	rBV3	35053	51216	1.40%	0.198%
11	9.969	1302	1306	1309	rBV	1422567	1108651	30.28%	4.287%
12	10.763	1436	1441	1444	rBV	2529879	2478933	67.71%	9.586%
13	11.457	1555	1559	1562	rBV	1310969	1170020	31.96%	4.525%
14	11.480	1562	1563	1566	rVV	248553	154136	4.21%	0.596%
15	11.533	1566	1572	1574	rVB	51238	72248	1.97%	0.279%
16	11.839	1621	1624	1627	rVB	102031	77331	2.11%	0.299%
17	11.975	1640	1647	1652	rBV3	67865	134696	3.68%	0.521%
18	12.075	1660	1664	1666	rBV2	39089	43830	1.20%	0.169%
19	12.669	1762	1765	1769	rBV	356926	324941	8.88%	1.257%
20	12.904	1798	1805	1808	rBV	308984	334298	9.13%	1.293%
21	13.045	1825	1829	1832	rBV	3522392	3357666	91.71%	12.984%
22	13.933	1976	1980	1990	rVB3	270559	365272	9.98%	1.413%
23	14.098	2000	2008	2011	rBV2	755373	847751	23.16%	3.278%
24	14.127	2011	2013	2020	rVB	127939	133003	3.63%	0.514%
25	14.251	2031	2034	2038	rBV	39981	41464	1.13%	0.160%
26	14.633	2093	2099	2100	rBV5	50438	89694	2.45%	0.347%
27	14.780	2120	2124	2126	rBV3	32851	44363	1.21%	0.172%
28	14.874	2137	2140	2146	rVB2	35178	42171	1.15%	0.163%
29	15.157	2184	2188	2191	rBV	88474	130855	3.57%	0.506%
30	15.221	2196	2199	2204	rVB4	32603	40951	1.12%	0.158%
31	15.468	2238	2241	2247	rVB	50209	65273	1.78%	0.252%
32	15.533	2249	2252	2256	rVV	65612	79670	2.18%	0.308%
33	15.604	2259	2264	2275	rBV	433343	584352	15.96%	2.260%
34	16.139	2352	2355	2362	rBV8	19492	42336	1.16%	0.164%
35	16.251	2368	2374	2378	rBV4	28873	74095	2.02%	0.287%
36	17.127	2517	2523	2529	rBV3	35769	72810	1.99%	0.282%

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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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.586	2596	2601	2609	rBV2	30051	67623	1.85%	0.262%
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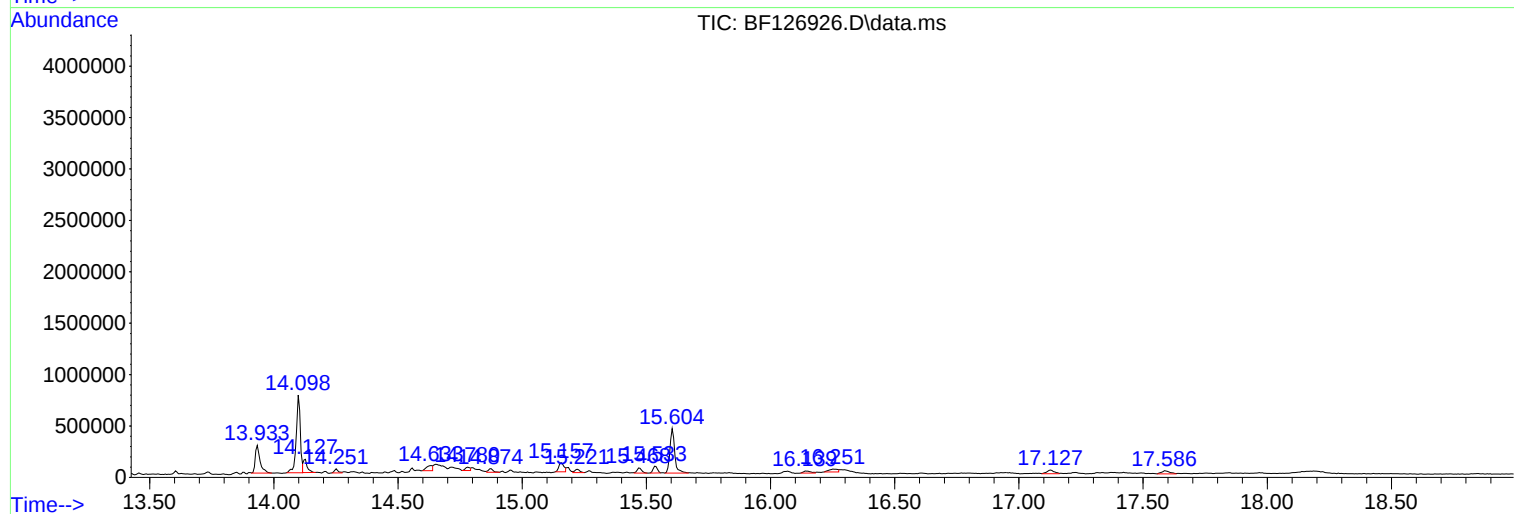
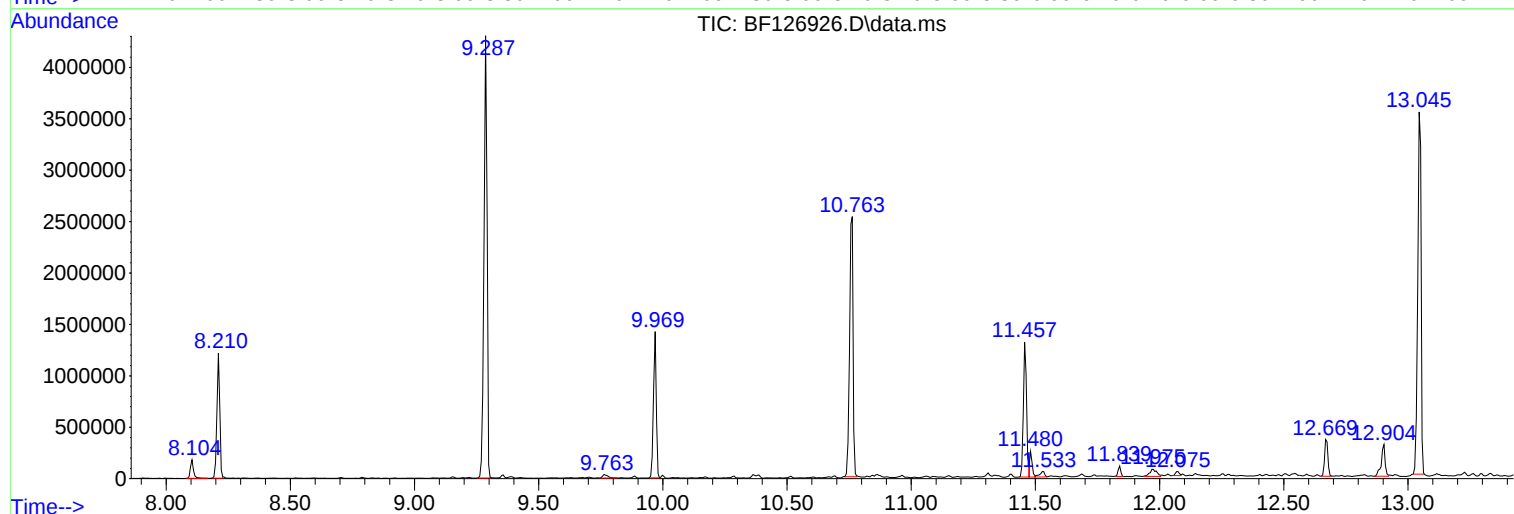
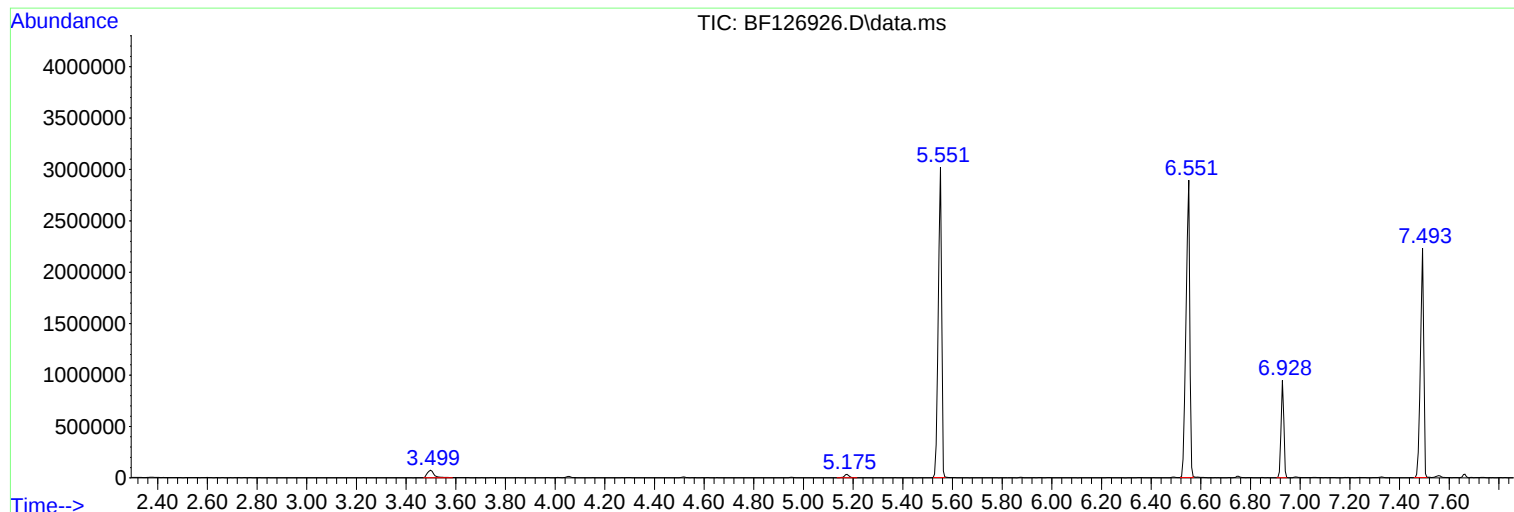
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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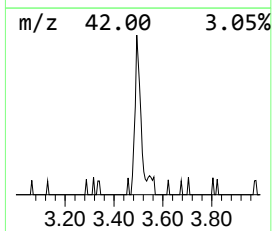
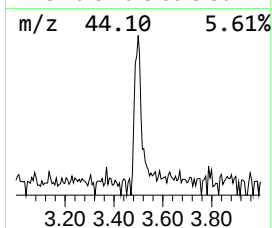
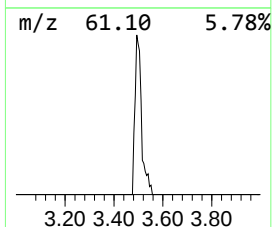
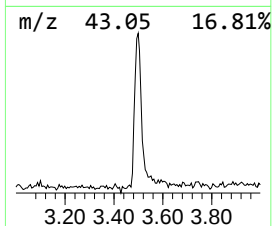
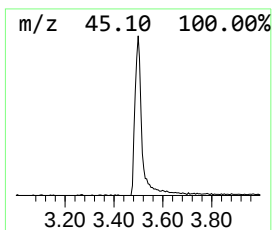
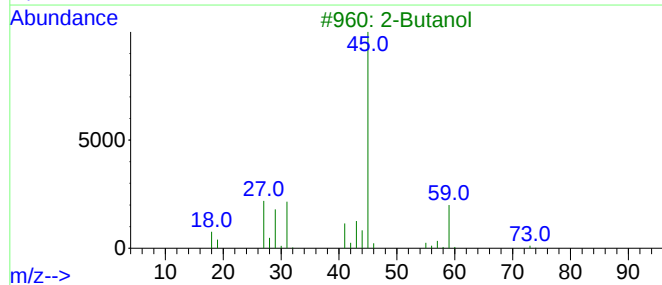
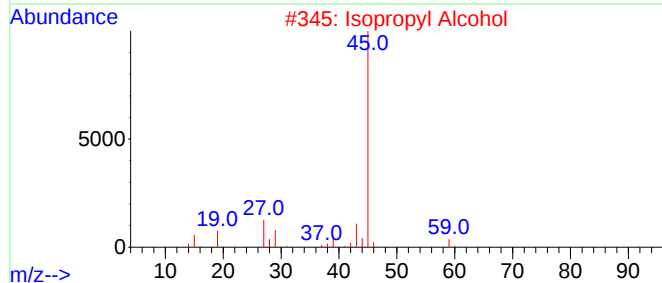
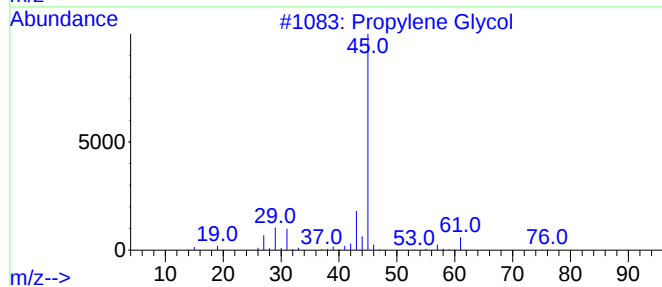
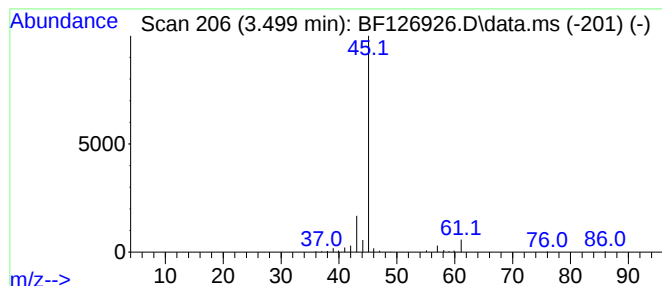
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.499	3.98 ng	143816	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	64
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	50
3			2-Butanol	74	C4H10O	000078-92-2	40
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



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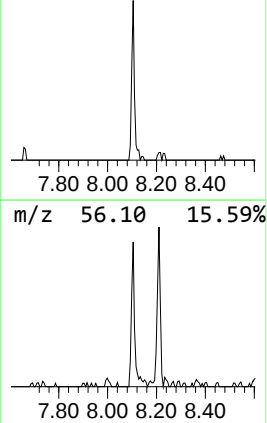
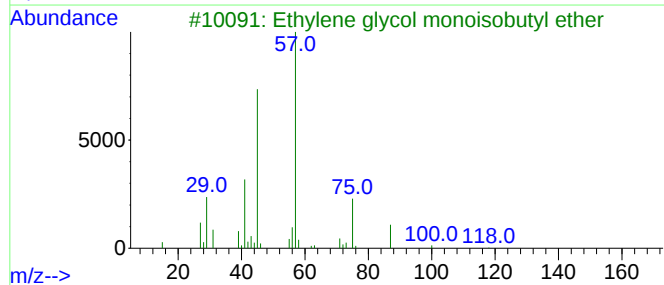
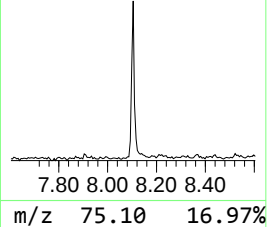
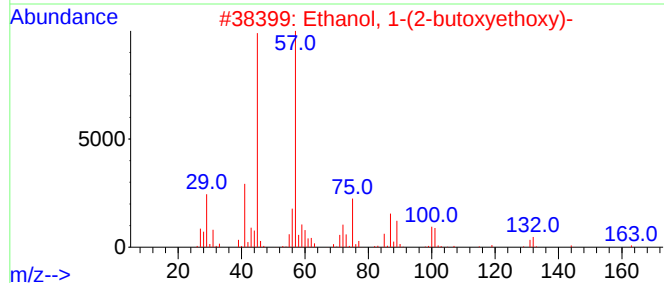
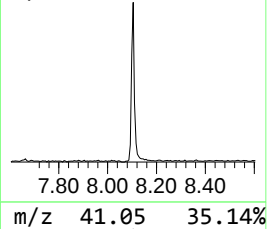
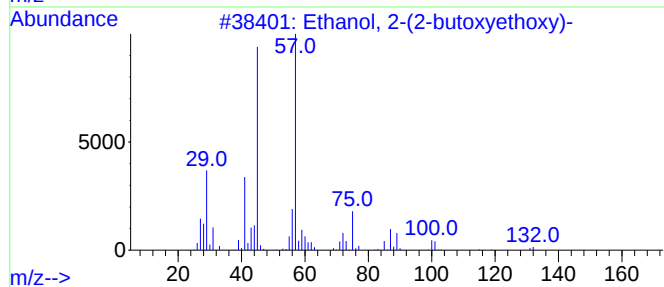
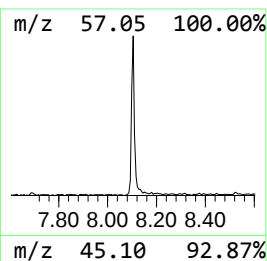
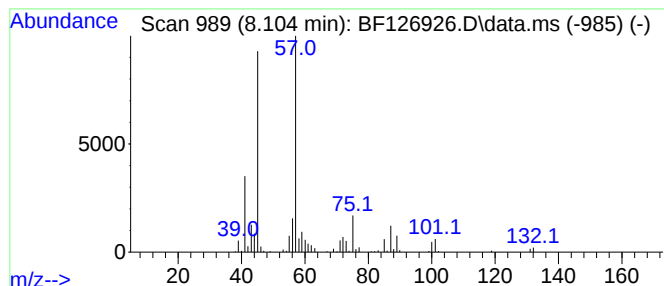
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	3.11 ng	153633	Naphthalene-d8	8.210

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			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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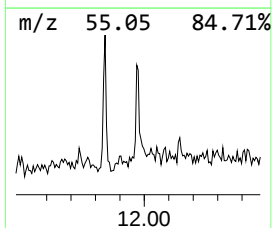
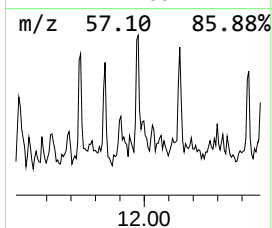
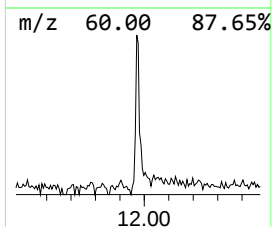
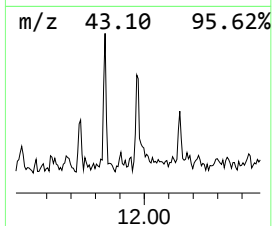
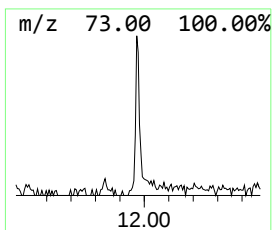
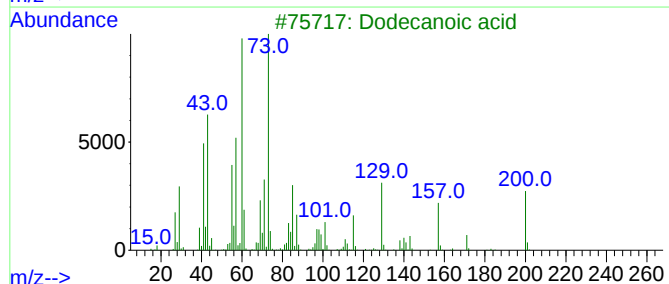
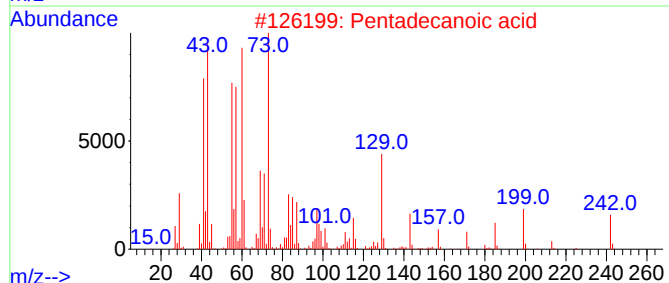
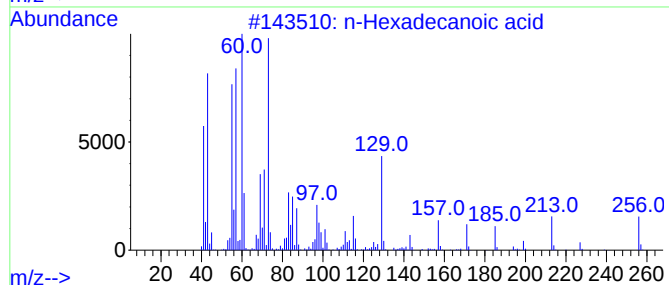
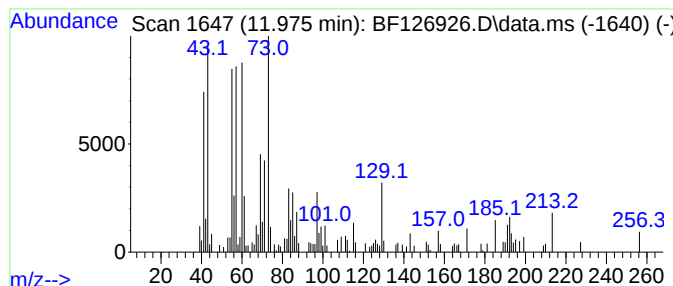
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.975	2.30 ng	134696	Phenanthrene-d10	11.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3			Dodecanoic acid	200	C12H24O2	000143-07-7	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Nonanoic acid	158	C9H18O2	000112-05-0	27



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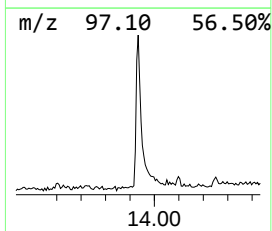
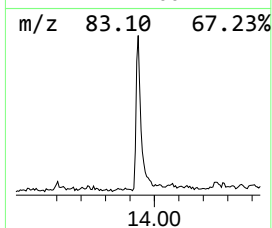
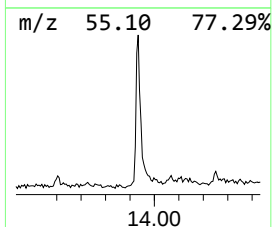
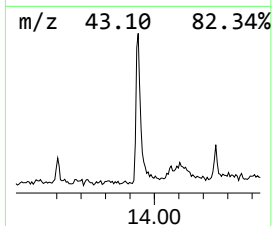
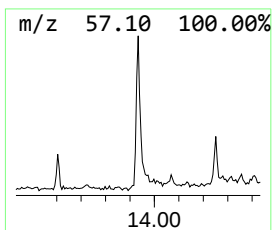
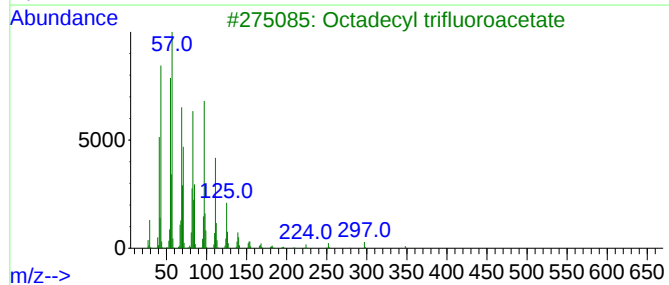
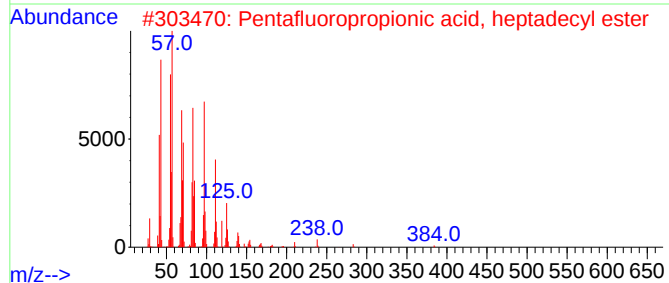
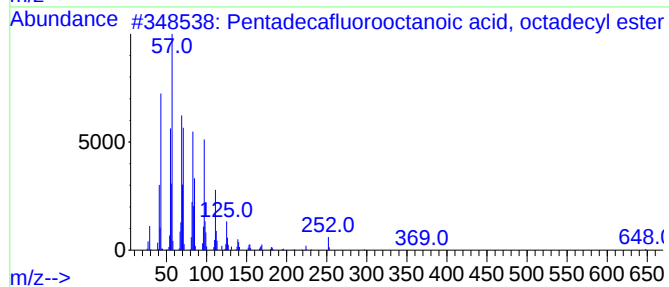
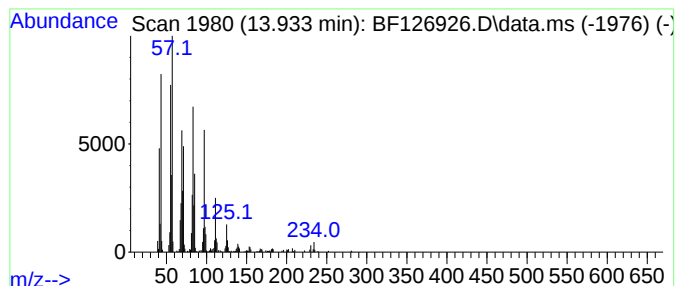
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	8.62 ng	365272	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91



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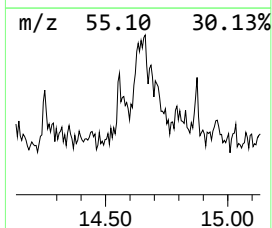
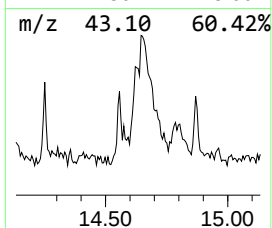
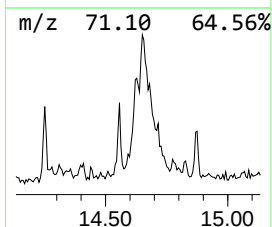
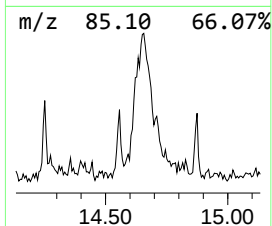
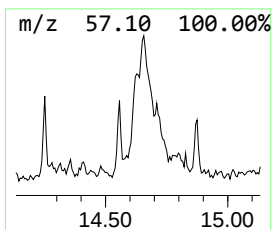
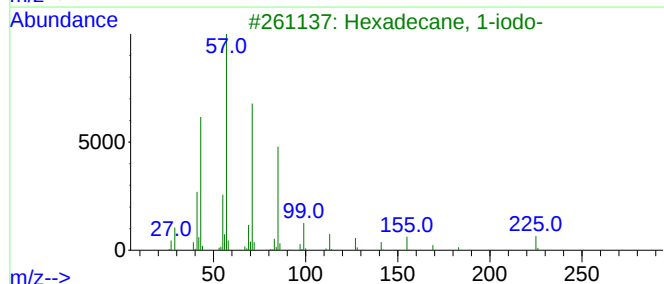
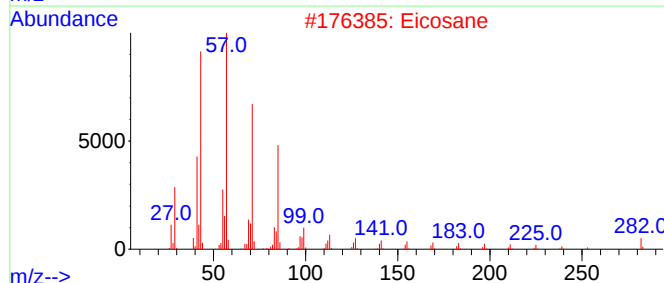
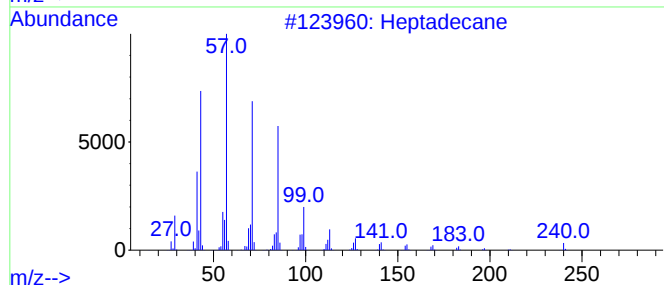
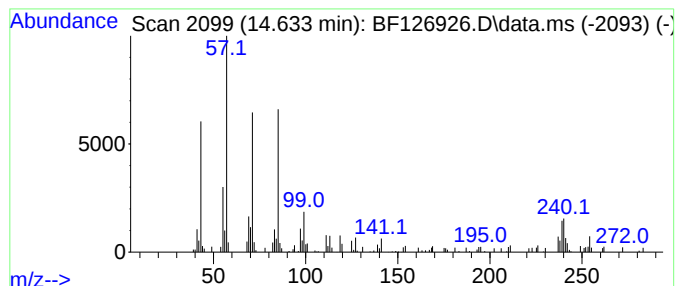
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	2.12 ng	89694	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	68
2			Eicosane	282	C20H42	000112-95-8	64
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	58
4			Heneicosane	296	C21H44	000629-94-7	58
5			Hexadecane	226	C16H34	000544-76-3	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126926.D
Acq On : 17 Feb 2022 14:52
Operator : CG\JU
Sample : N1564-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

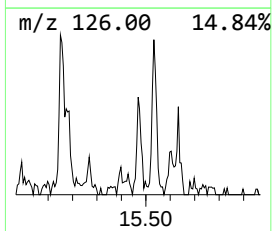
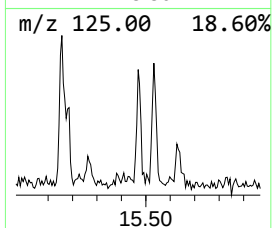
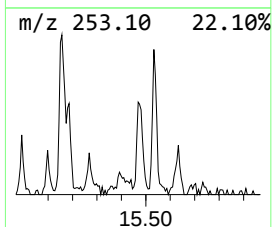
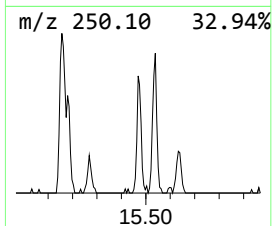
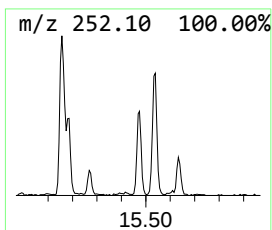
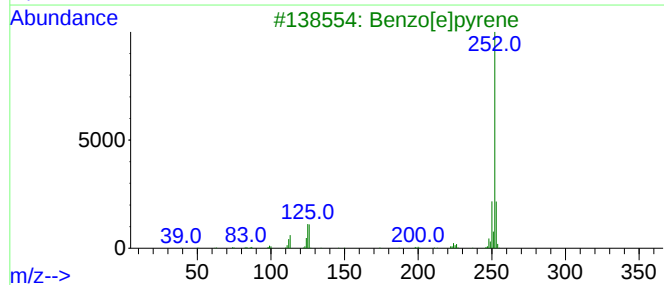
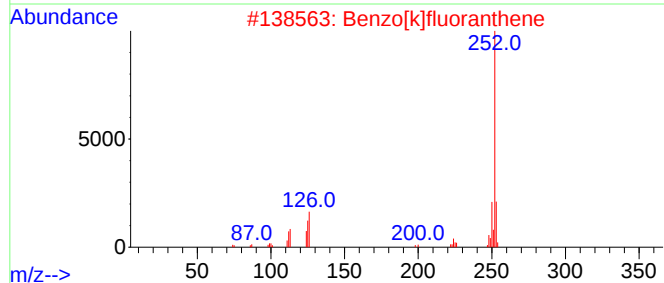
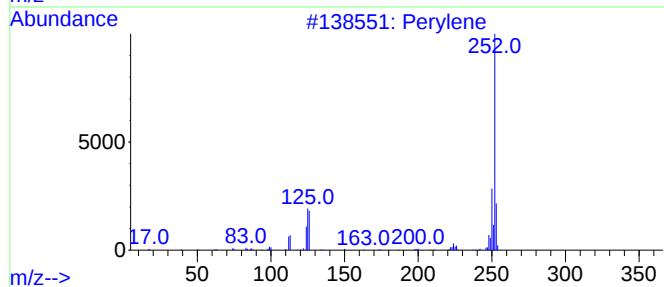
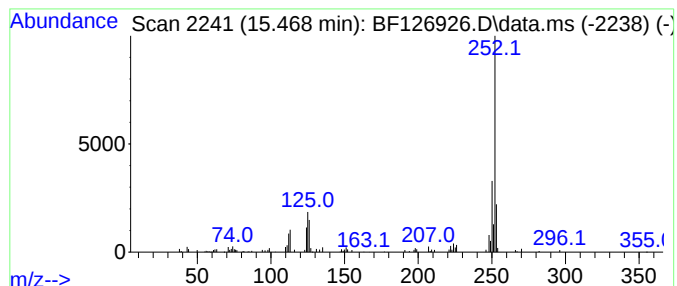
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Perylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.469	2.23 ng	65273	Perylene-d12	15.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3			Benzo[e]pyrene	252	C20H12	000192-97-2	95
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126926.D
Acq On : 17 Feb 2022 14:52
Operator : CG\JU
Sample : N1564-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

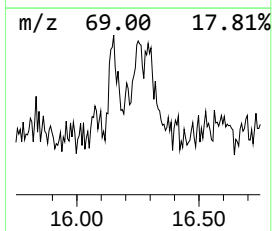
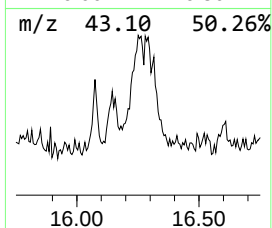
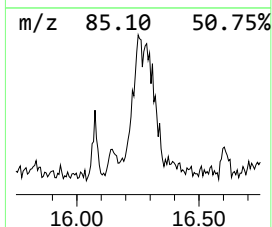
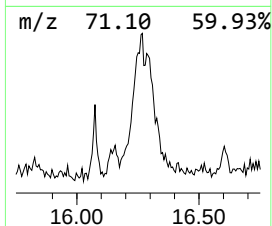
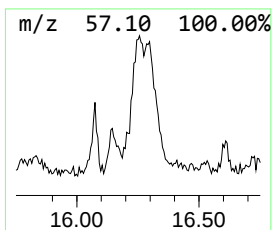
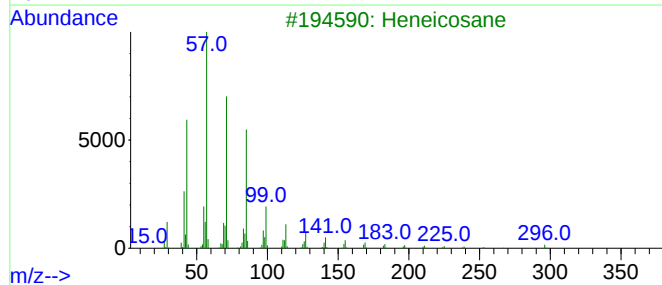
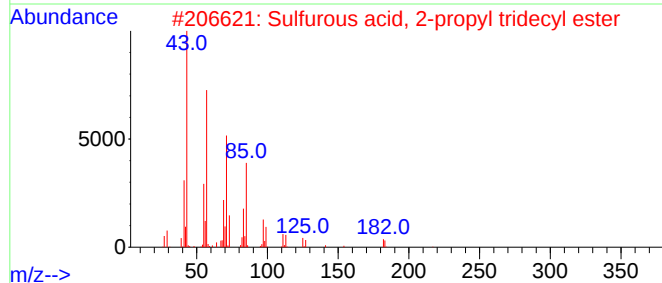
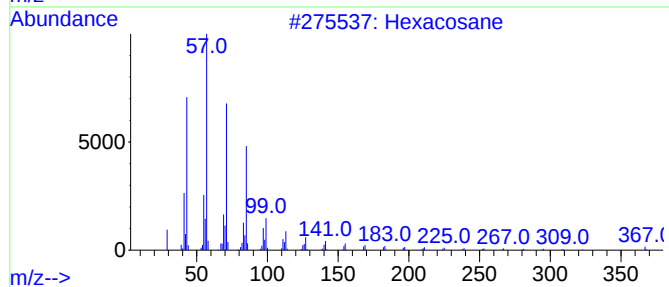
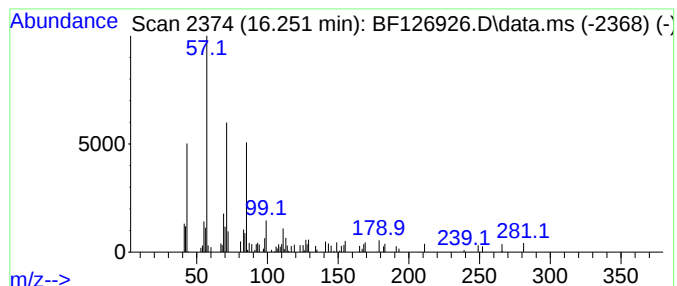
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.251	2.54 ng	74095	Perylene-d12	15.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	72
2			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	72
3			Heneicosane	296	C21H44	000629-94-7	72
4			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	72
5			Heptadecane	240	C17H36	000629-78-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126926.D
Acq On : 17 Feb 2022 14:52
Operator : CG\JU
Sample : N1564-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
Propylene Glycol	3.499	4.0	ng	143816	1	6.928	722817	20.0
Ethanol, 2-(2-b...	8.104	3.1	ng	153633	2	8.210	988432	20.0
n-Hexadecanoic ...	11.975	2.3	ng	134696	4	11.457	1170020	20.0
Pentadecafluoro...	13.933	8.6	ng	365272	5	14.098	847751	20.0
Heptadecane	14.633	2.1	ng	89694	5	14.098	847751	20.0
Perylene	15.469	2.2	ng	65273	6	15.604	584352	20.0
Hexacosane	16.251	2.5	ng	74095	6	15.604	584352	20.0