

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
 Data File : BF126049.D
 Acq On : 4 Nov 2021 17:00
 Operator : JU/CG
 Sample : M4500-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-8-110321

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126049.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	21	rVB	1429602	1808434	63.12%	7.401%
2	3.316	206	209	219	rBV	79465	193484	6.75%	0.792%
3	5.063	503	506	511	rVB	94343	109347	3.82%	0.447%
4	5.469	570	575	578	rBV	2957124	2728956	95.24%	11.168%
5	6.475	741	746	749	rBV	2944884	2688002	93.81%	11.000%
6	6.851	807	810	814	rBV	1031672	794372	27.72%	3.251%
7	7.410	900	905	908	rBV	2022857	1742707	60.82%	7.132%
8	8.033	1008	1011	1023	rBV	211899	210467	7.35%	0.861%
9	8.133	1023	1028	1031	rBV	1127084	895652	31.26%	3.665%
10	9.157	1200	1202	1206	rVB2	53986	46305	1.62%	0.189%
11	9.210	1206	1211	1214	rBV	3713532	2865236	100.00%	11.725%
12	9.292	1222	1225	1229	rBV2	46263	55552	1.94%	0.227%
13	9.469	1252	1255	1260	rBV3	37947	52585	1.84%	0.215%
14	9.545	1262	1268	1270	rBV2	53479	57488	2.01%	0.235%
15	9.616	1275	1280	1282	rBV3	50635	59921	2.09%	0.245%
16	9.663	1285	1288	1293	rVV2	31382	38707	1.35%	0.158%
17	9.745	1300	1302	1307	rVB	49178	40821	1.42%	0.167%
18	9.886	1319	1326	1329	rBV	1061909	859969	30.01%	3.519%
19	9.916	1329	1331	1335	rVB	50263	51423	1.79%	0.210%
20	10.086	1357	1360	1363	rVB4	54863	49909	1.74%	0.204%
21	10.204	1374	1380	1383	rBV4	34716	50534	1.76%	0.207%
22	10.427	1415	1418	1424	rVB4	49152	61738	2.15%	0.253%
23	10.669	1455	1459	1464	rBV	1823506	1506262	52.57%	6.164%
24	10.792	1477	1480	1482	rBV4	49067	56930	1.99%	0.233%
25	11.239	1551	1556	1558	rBV5	40288	42838	1.50%	0.175%
26	11.268	1558	1561	1567	rVB2	63733	73792	2.58%	0.302%
27	11.368	1574	1578	1580	rBV	958367	774469	27.03%	3.169%
28	11.392	1580	1582	1585	rVV	187513	134684	4.70%	0.551%
29	11.439	1587	1590	1594	rVB	102823	105156	3.67%	0.430%
30	11.480	1594	1597	1600	rBV5	25308	38363	1.34%	0.157%
31	11.768	1642	1646	1653	rVB2	73029	86178	3.01%	0.353%
32	11.868	1660	1663	1666	rBV	71411	77124	2.69%	0.316%
33	11.898	1666	1668	1670	rVB	89728	68350	2.39%	0.280%
34	11.980	1679	1682	1685	rBV	115293	125918	4.39%	0.515%
35	12.074	1696	1698	1701	rBV	46505	35726	1.25%	0.146%
36	12.357	1742	1746	1751	rBV6	34308	63425	2.21%	0.260%

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Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

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37	12.421	1754	1757	1760	rBV3	75353	81323	2.84%	0.333%
38	12.474	1760	1766	1769	rVB4	127899	236915	8.27%	0.970%
39	12.580	1781	1784	1787	rVB	241357	191427	6.68%	0.783%
40	12.810	1820	1823	1825	rVV	256544	208941	7.29%	0.855%
41	12.833	1825	1827	1829	rVB2	71716	52608	1.84%	0.215%
42	12.957	1844	1848	1851	rBV	3189272	2835978	98.98%	11.606%
43	13.192	1886	1888	1892	rVB3	66029	85028	2.97%	0.348%
44	13.239	1894	1896	1899	rBV	50222	43153	1.51%	0.177%
45	13.533	1944	1946	1949	rBV2	81968	79435	2.77%	0.325%
46	13.862	1999	2002	2013	rVB	245020	346971	12.11%	1.420%
47	14.004	2022	2026	2029	rBV	994044	964758	33.67%	3.948%
48	14.486	2106	2108	2110	rBV	105481	93103	3.25%	0.381%
49	15.468	2272	2275	2279	rBV	524426	565946	19.75%	2.316%

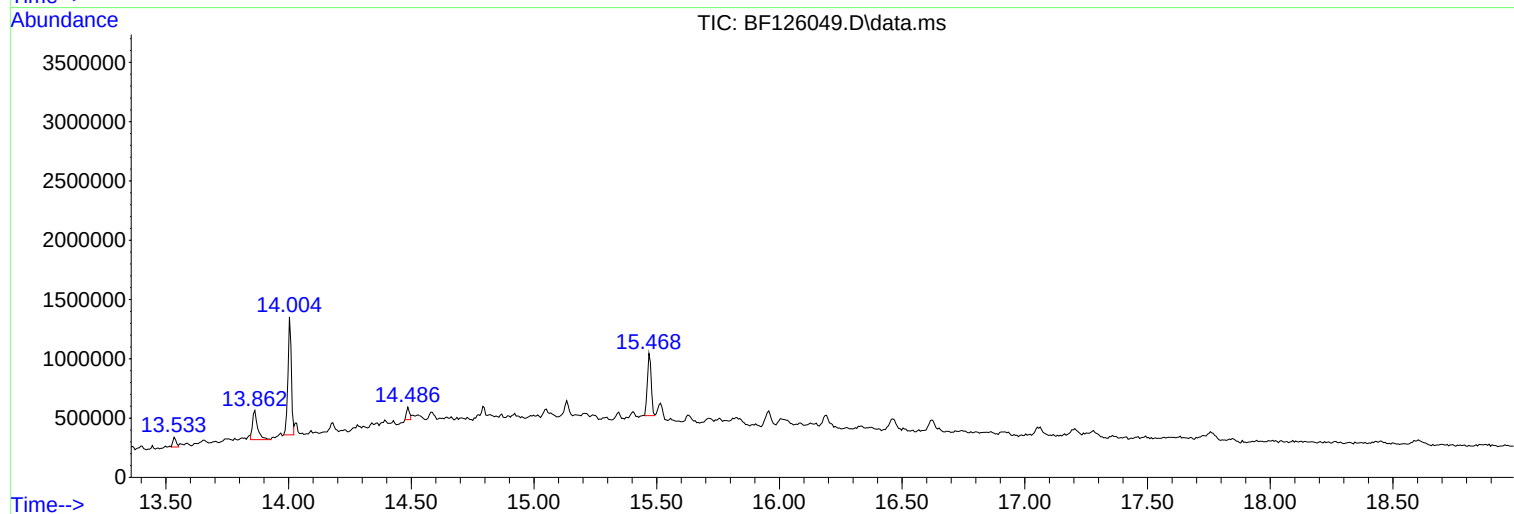
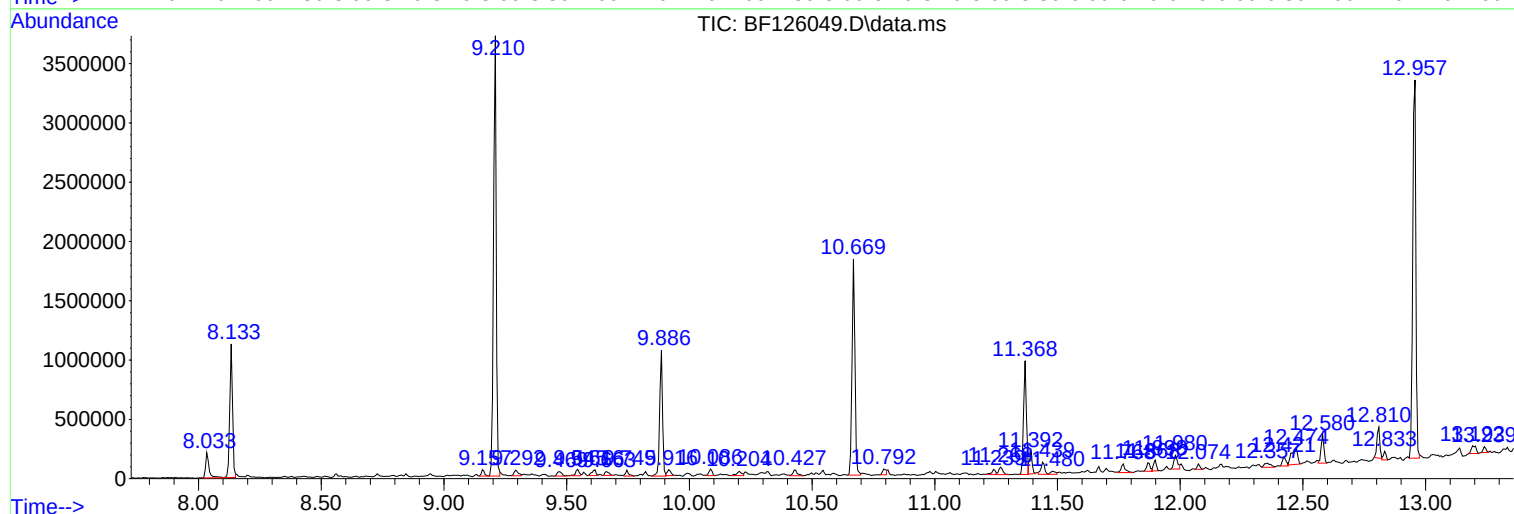
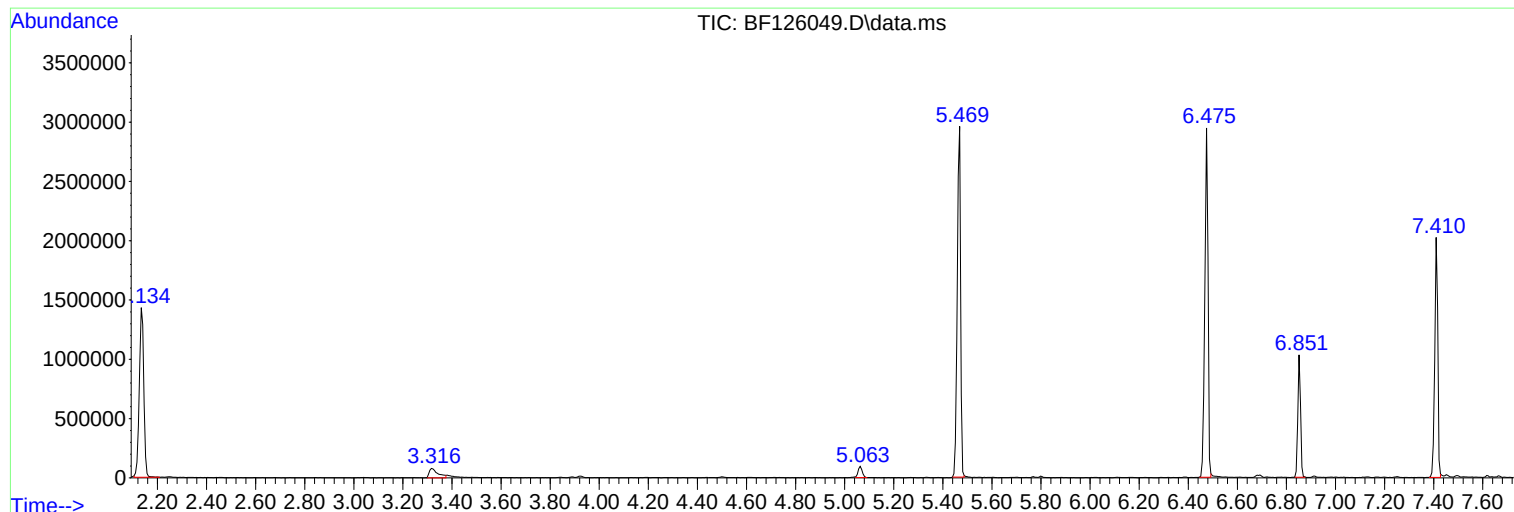
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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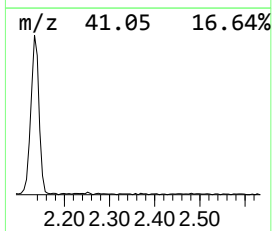
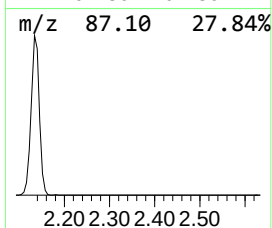
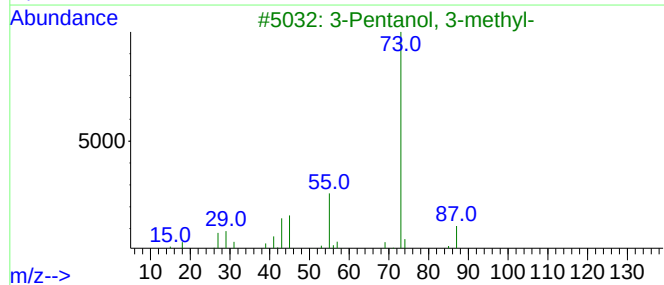
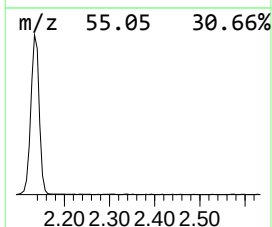
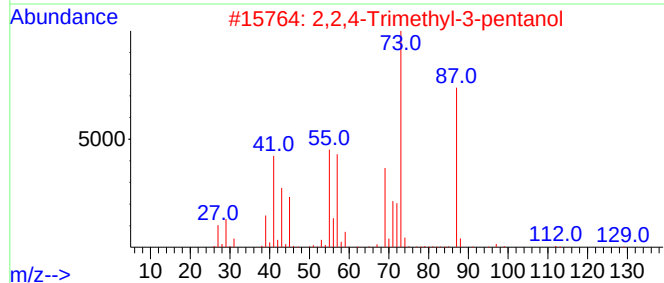
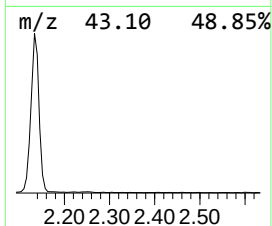
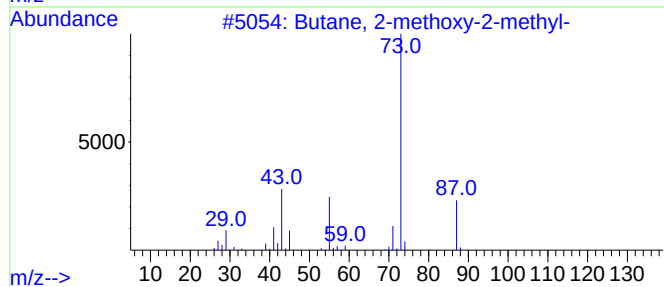
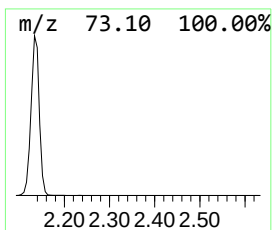
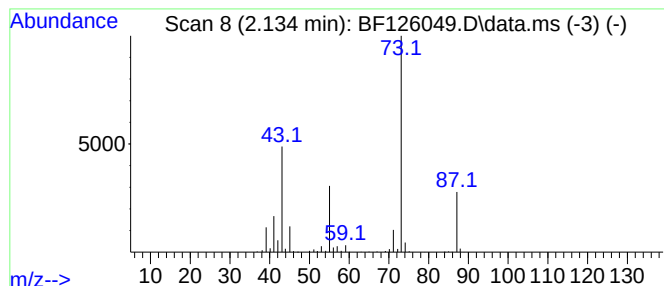
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	45.53 ng	1808430	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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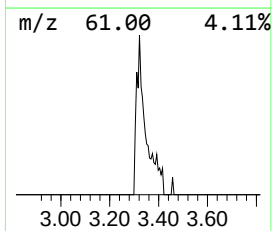
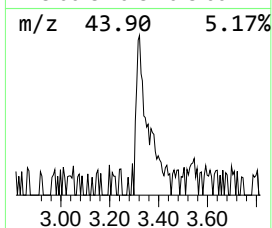
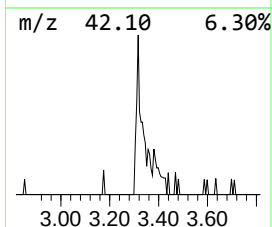
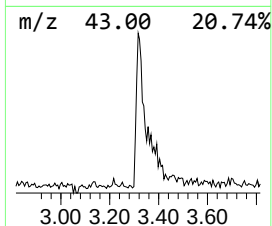
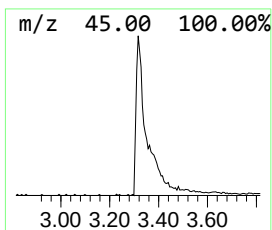
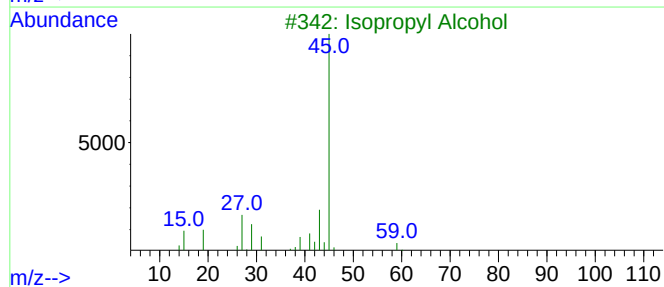
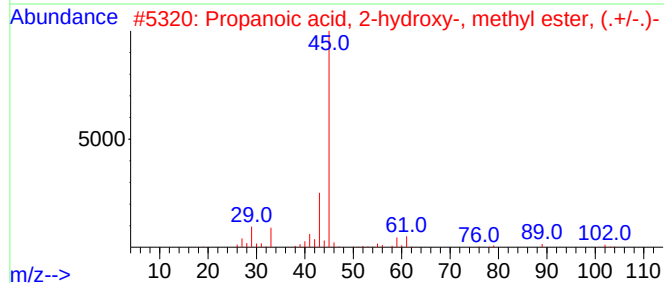
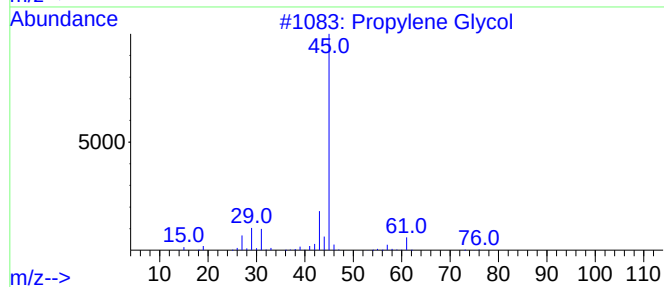
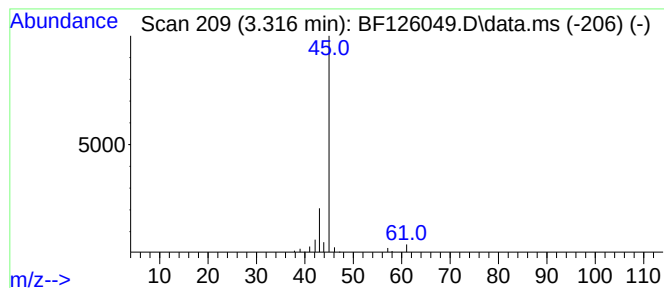
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.316	4.87 ng	193484	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	64
2			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	4
5			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4



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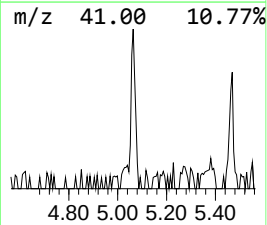
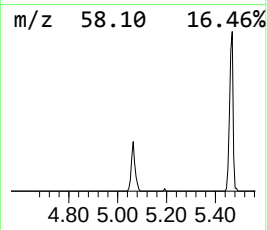
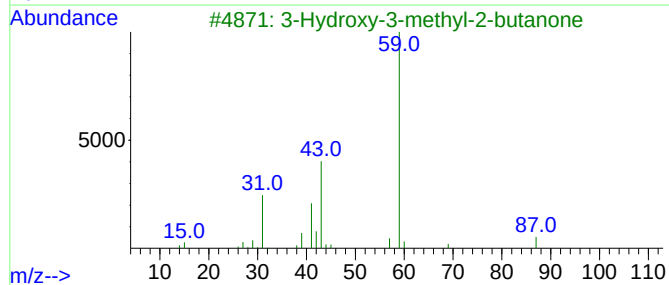
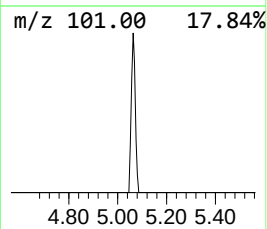
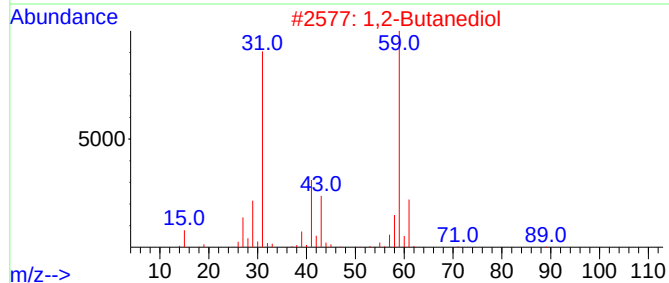
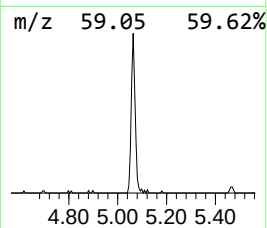
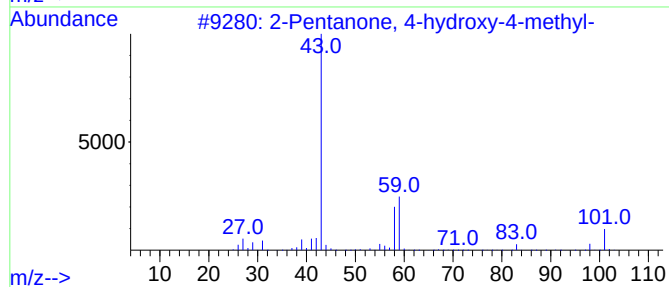
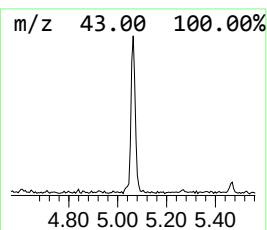
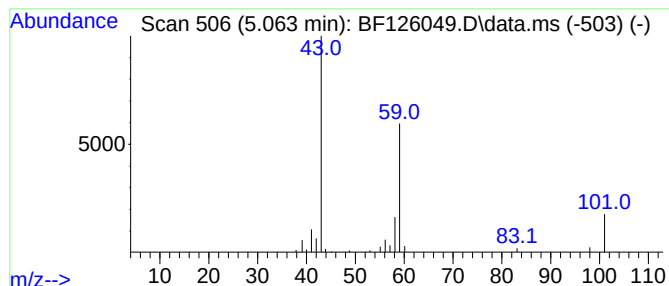
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	2.75 ng	109347	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	1,2-Butanediol	90	C4H10O2	000584-03-2	38		
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	37		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	16		



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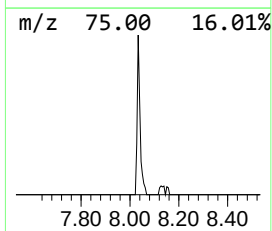
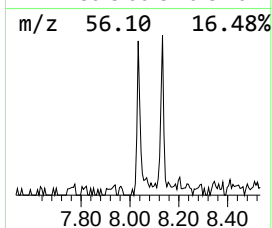
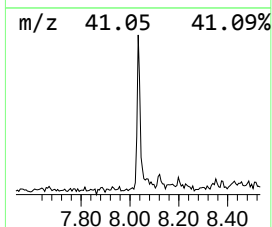
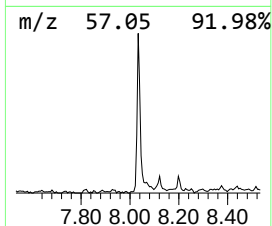
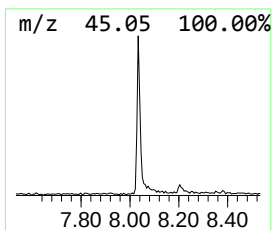
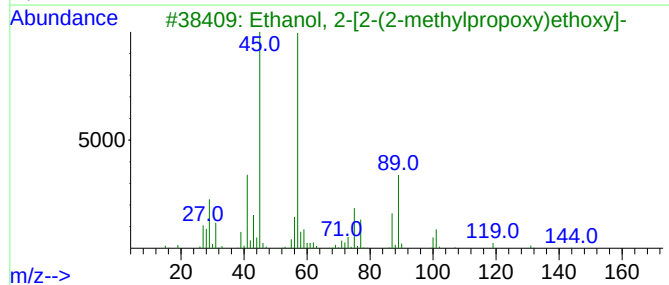
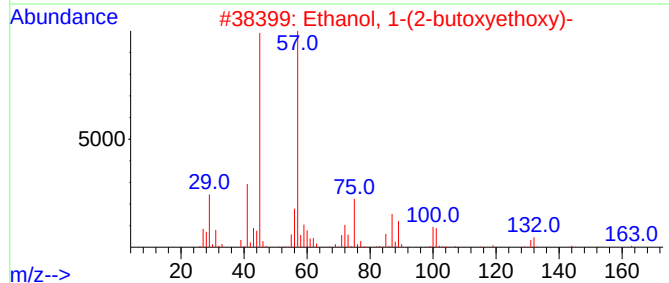
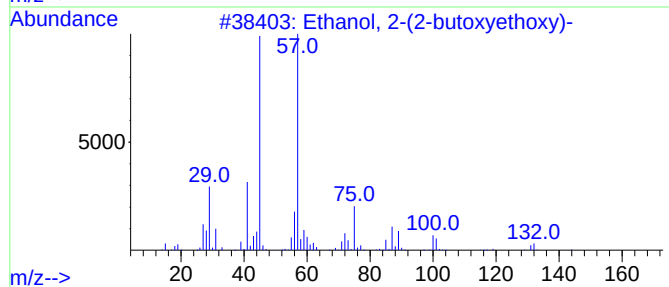
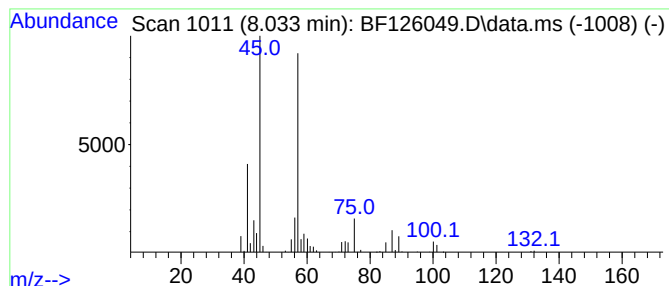
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.033	4.70 ng	210467	Naphthalene-d8	8.133

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	56
4			2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	53
5			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	53



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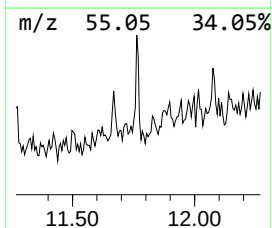
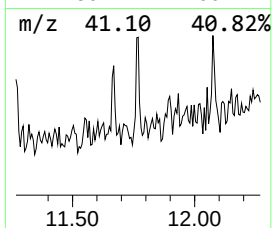
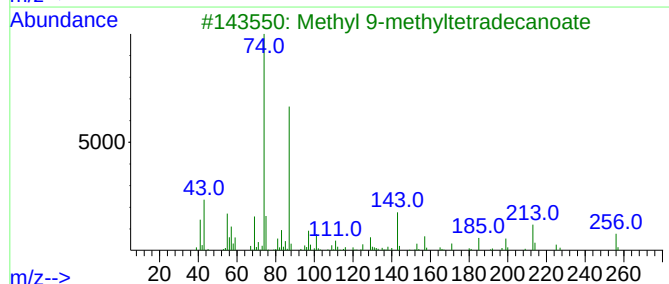
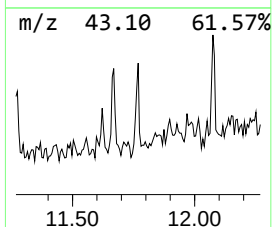
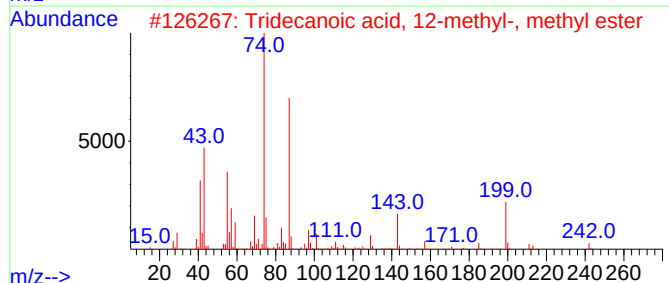
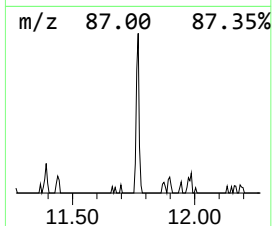
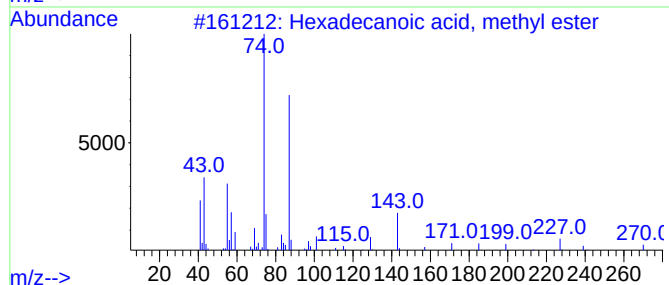
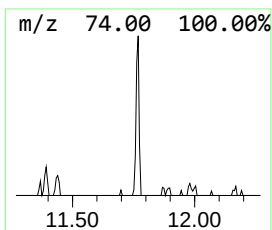
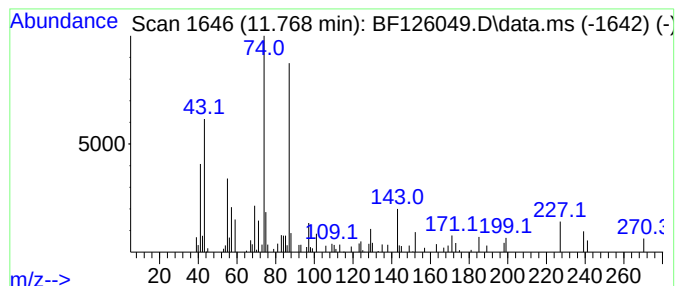
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.769	2.23 ng	86178	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80
3			Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	64
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	64
5			Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126049.D
Acq On : 4 Nov 2021 17:00
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

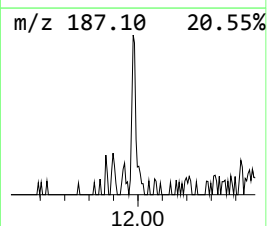
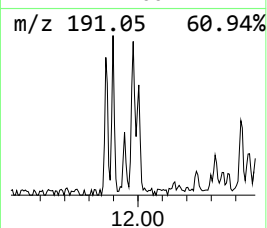
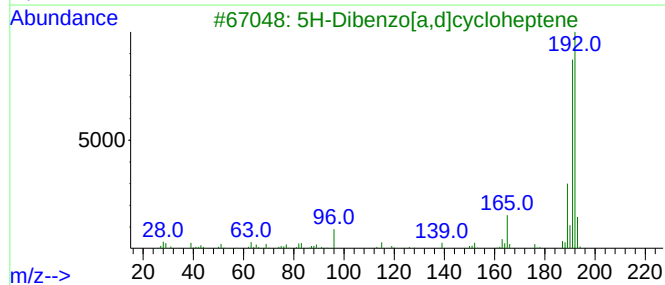
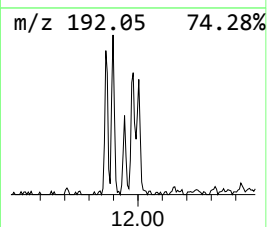
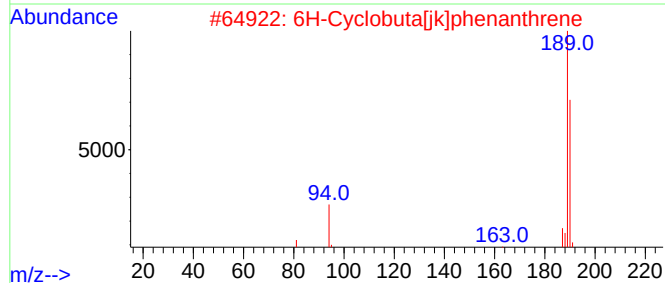
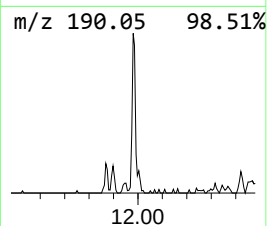
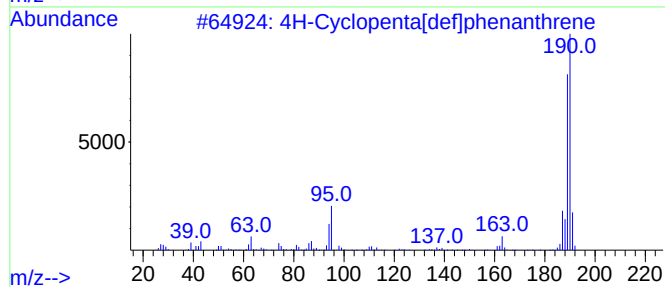
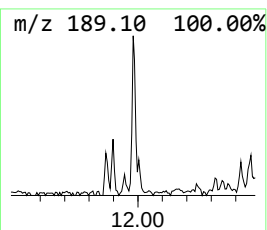
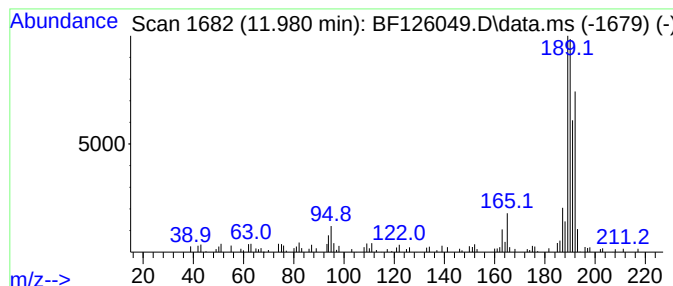
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	3.25 ng	125918	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	46
4			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	43
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126049.D
Acq On : 4 Nov 2021 17:00
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

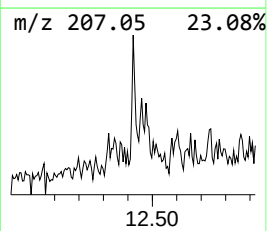
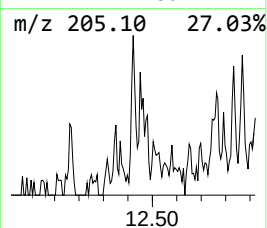
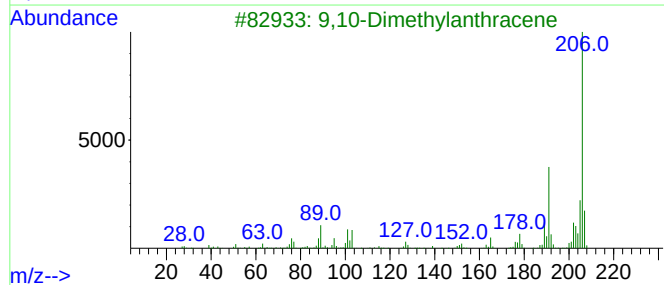
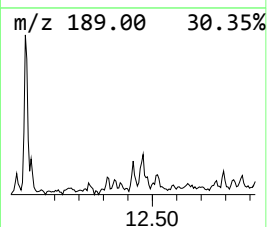
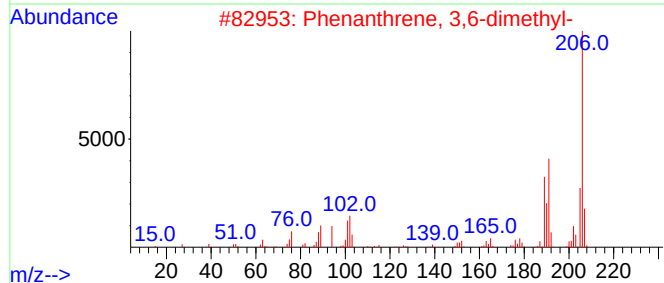
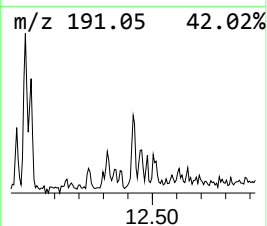
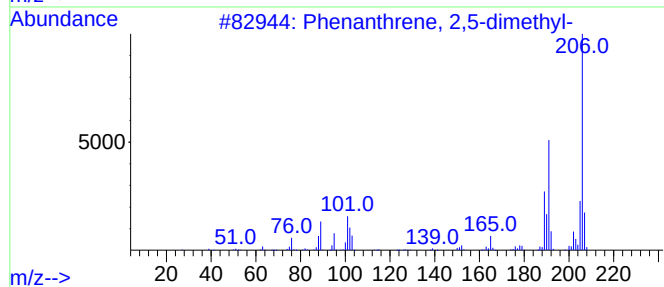
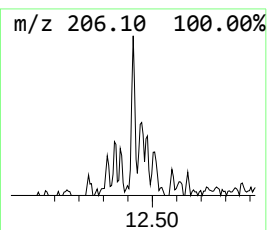
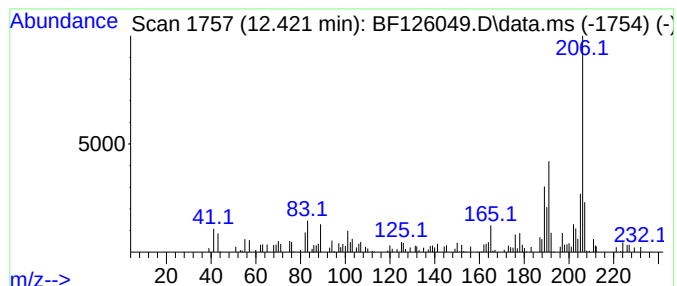
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	2.10 ng	81323	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
2			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90
3			9,10-Dimethylanthracene	206	C16H14	000781-43-1	90
4			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	90
5			Anthracene, 2-ethyl-	206	C16H14	052251-71-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126049.D
Acq On : 4 Nov 2021 17:00
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

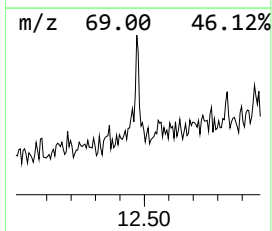
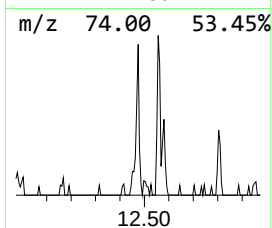
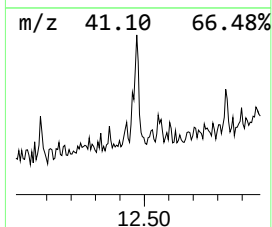
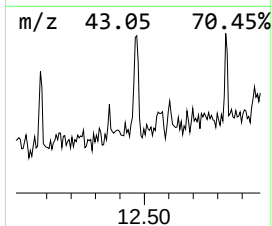
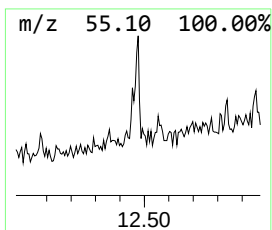
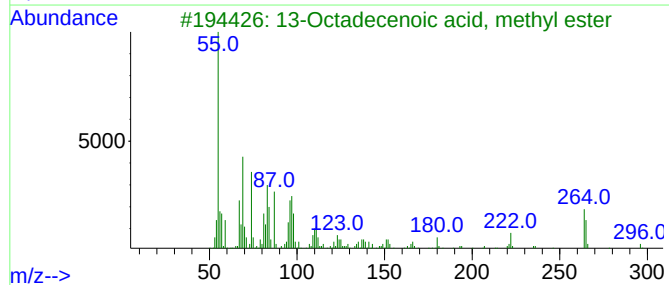
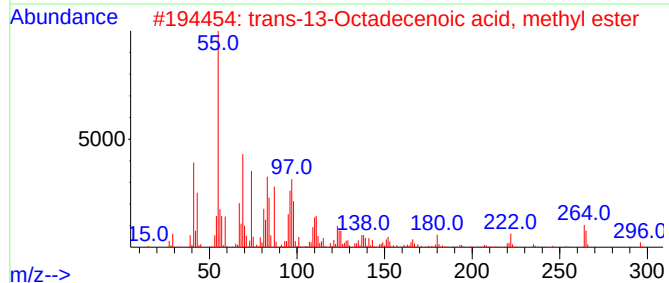
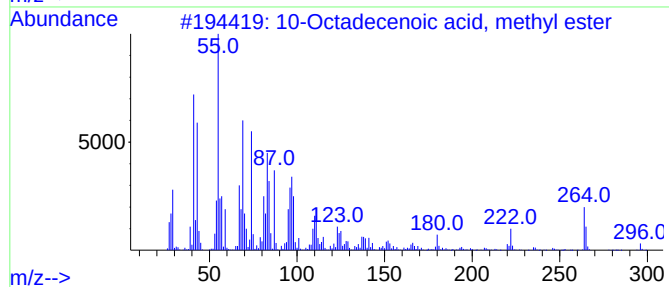
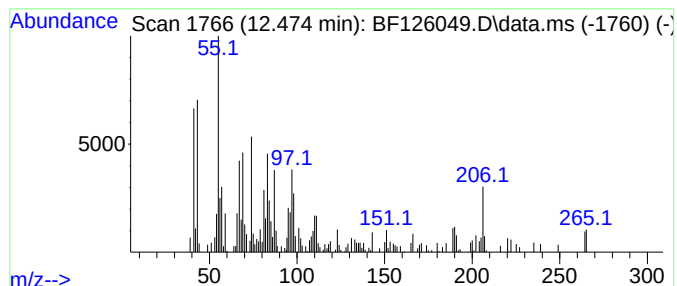
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 10-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.474	6.12 ng	236915	Phenanthrene-d10	11.368

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	81
2		trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	76
3		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	72
4		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	52
5		9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126049.D
Acq On : 4 Nov 2021 17:00
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

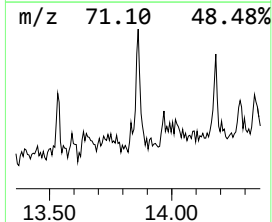
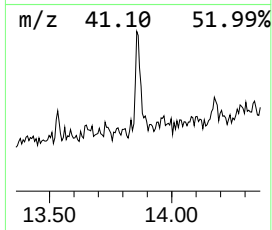
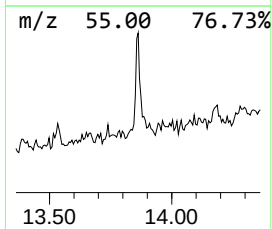
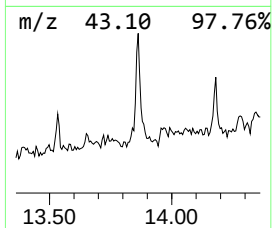
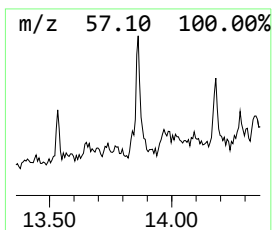
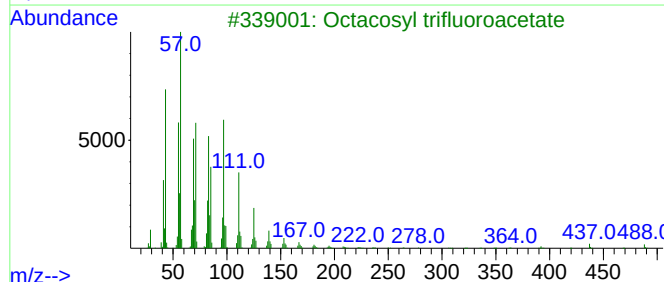
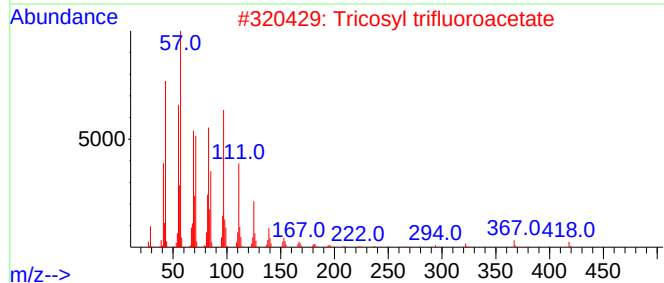
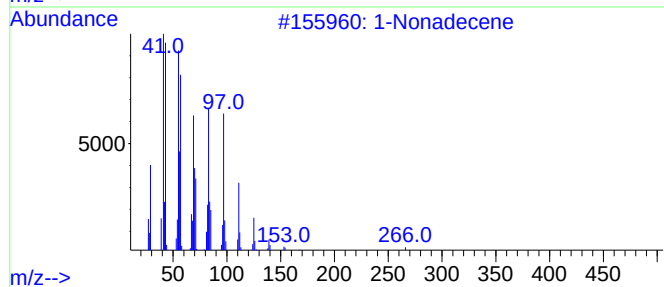
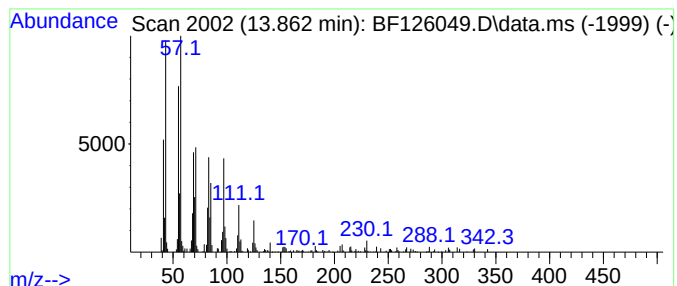
Instrument :
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ClientSampleId :
TR-8-110321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Nonadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.862	7.19 ng	346971	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	95
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
5	Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126049.D
Acq On : 4 Nov 2021 17:00
Operator : JU/CG
Sample : M4500-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-8-110321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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...	2.134	45.5	ng	1808430	1	6.851	794372	20.0
Propylene Glycol	3.316	4.9	ng	193484	1	6.851	794372	20.0
2-Pentanone, 4-...	5.063	2.8	ng	109347	1	6.851	794372	20.0
Ethanol, 2-(2-b...	8.033	4.7	ng	210467	2	8.133	895652	20.0
Hexadecanoic ac...	11.769	2.2	ng	86178	4	11.368	774469	20.0
4H-Cyclopenta[d...	11.980	3.3	ng	125918	4	11.368	774469	20.0
Phenanthrene, 2...	12.421	2.1	ng	81323	4	11.368	774469	20.0
10-Octadecenoic...	12.474	6.1	ng	236915	4	11.368	774469	20.0
1-Nonadecene	13.862	7.2	ng	346971	5	14.004	964758	20.0