

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041822\
 Data File : BF127825.D
 Acq On : 18 Apr 2022 15:12
 Operator : CG\JU
 Sample : N2442-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 124042

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-BF040622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127825.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.334	3	8	15	rVB	190669	254430	5.39%	0.730%
2	3.681	216	237	240	rBV	398491	1706061	36.13%	4.898%
3	5.581	555	560	563	rBV	3649482	3771835	79.89%	10.829%
4	6.575	723	729	732	rBV	3387765	3882164	82.22%	11.145%
5	6.945	789	792	796	rBV	1069834	974086	20.63%	2.796%
6	7.510	882	888	891	rBV	2380203	2655996	56.25%	7.625%
7	8.234	1006	1011	1014	rBV	1353643	1261858	26.73%	3.623%
8	9.310	1188	1194	1197	rBV	4691578	4470875	94.69%	12.835%
9	9.992	1303	1310	1313	rBV	1750625	1522468	32.25%	4.371%
10	10.022	1313	1315	1319	rVB	158095	118172	2.50%	0.339%
11	10.192	1340	1344	1348	rBV	65500	60495	1.28%	0.174%
12	10.539	1399	1403	1408	rVB	125151	103212	2.19%	0.296%
13	10.786	1438	1445	1448	rBV	3262163	3276687	69.40%	9.407%
14	11.486	1559	1564	1566	rBV	1664027	1633472	34.60%	4.690%
15	11.504	1566	1567	1571	rVB	437038	321082	6.80%	0.922%
16	12.004	1649	1652	1660	rVB3	119576	168541	3.57%	0.484%
17	12.098	1664	1668	1670	rBV	80139	72550	1.54%	0.208%
18	12.204	1681	1686	1696	rVB7	44146	111774	2.37%	0.321%
19	12.698	1766	1770	1774	rVB	455717	375647	7.96%	1.078%
20	12.927	1803	1809	1812	rBV	306449	327586	6.94%	0.940%
21	13.075	1829	1834	1837	rVB	5075622	4721491	100.00%	13.555%
22	13.322	1872	1876	1879	rBV	46297	49355	1.05%	0.142%
23	13.992	1985	1990	2005	rVB2	193334	485515	10.28%	1.394%
24	14.127	2009	2013	2016	rVV	1230214	1165682	24.69%	3.347%
25	14.151	2016	2017	2024	rVB	77832	64641	1.37%	0.186%
26	14.227	2025	2030	2035	rVV	104472	131253	2.78%	0.377%
27	14.439	2062	2066	2071	rBV7	33952	51043	1.08%	0.147%
28	14.751	2116	2119	2122	rBV	165063	156072	3.31%	0.448%
29	15.192	2191	2194	2198	rBV	40545	60105	1.27%	0.173%
30	15.645	2266	2271	2279	rBV	633907	878247	18.60%	2.521%

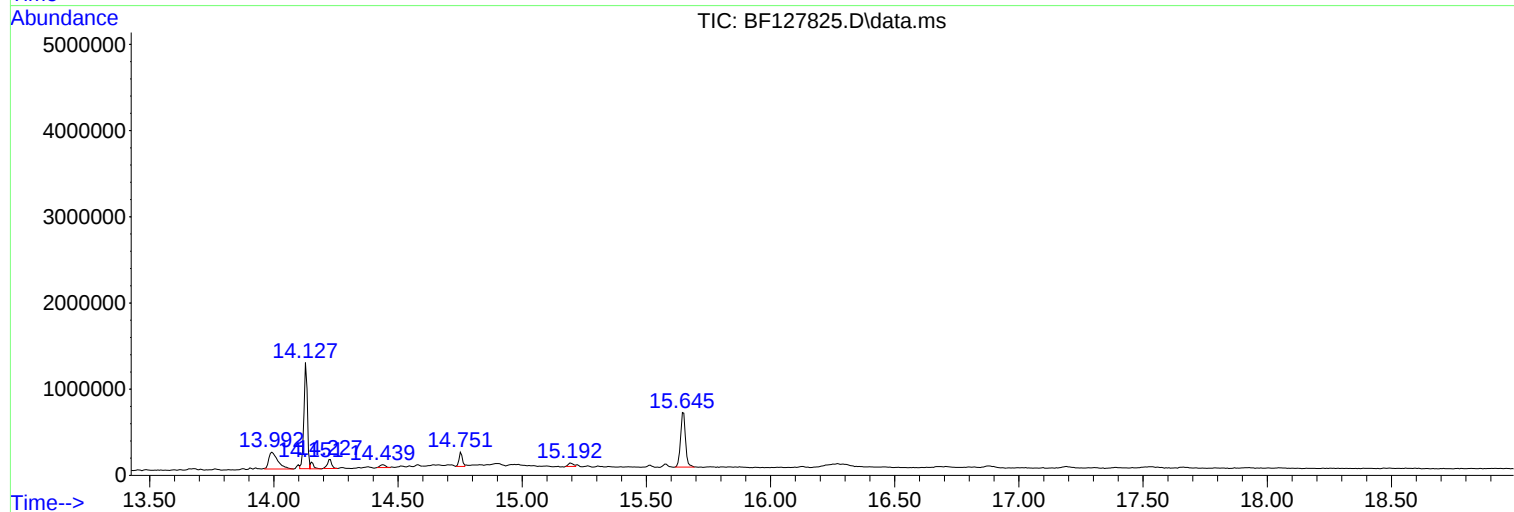
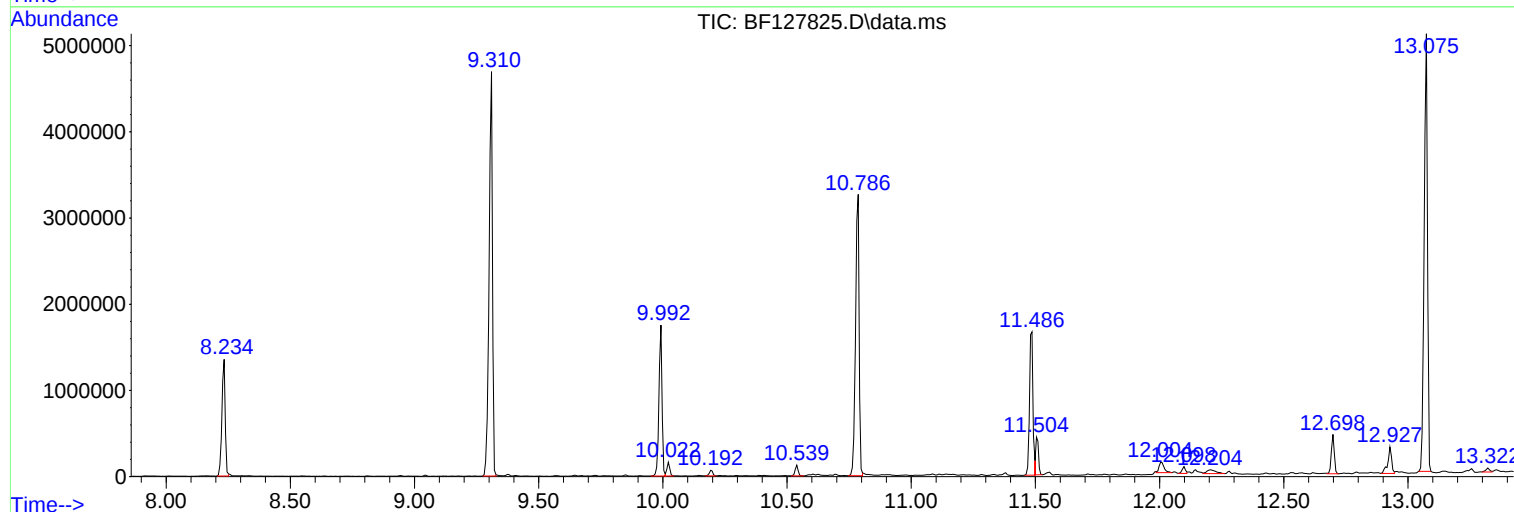
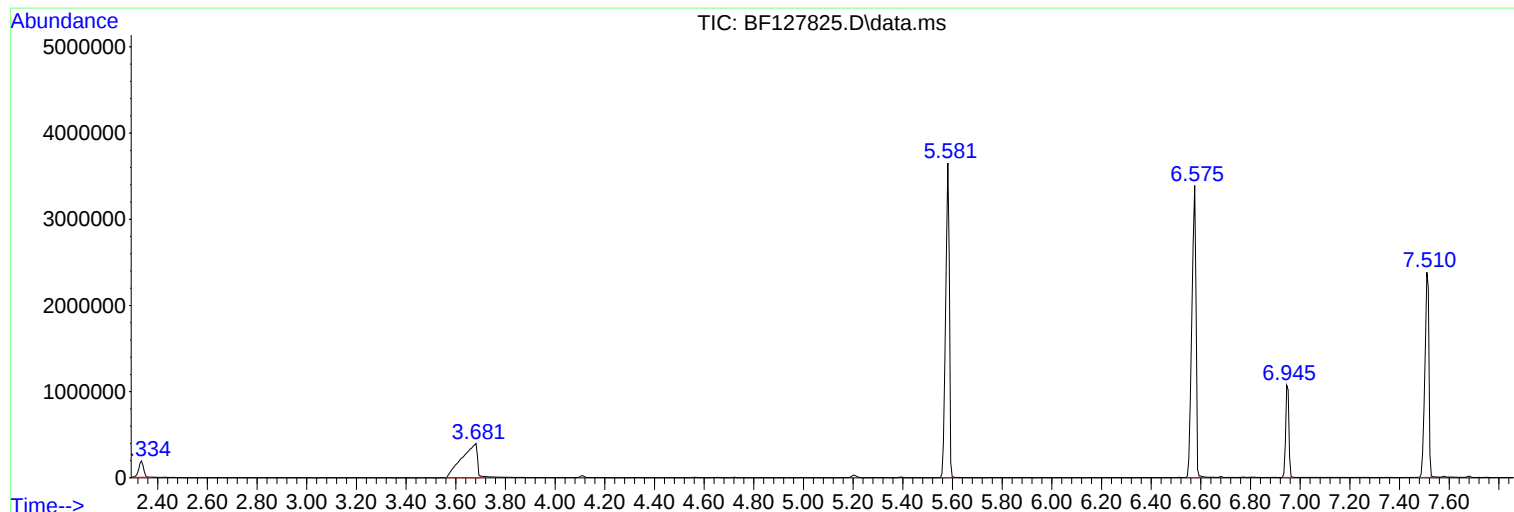
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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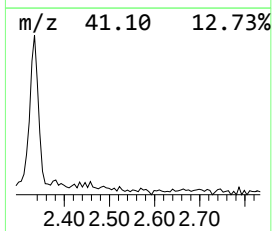
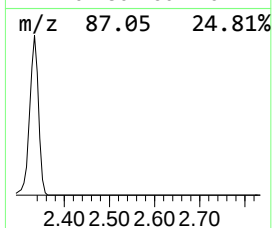
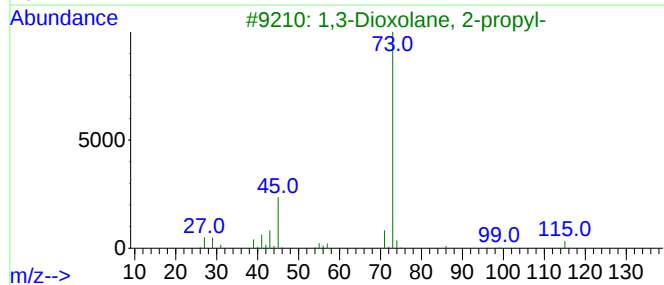
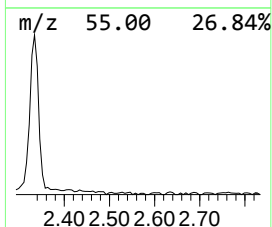
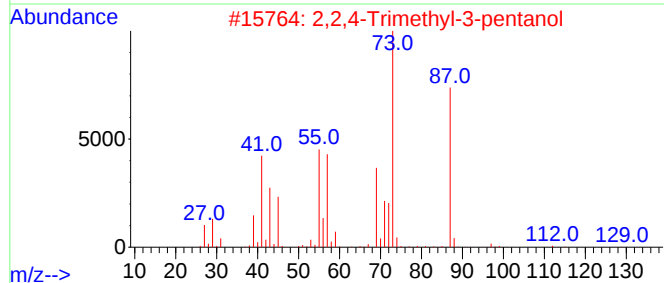
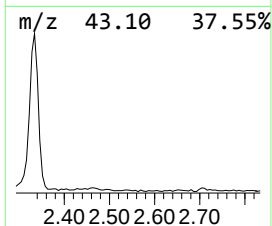
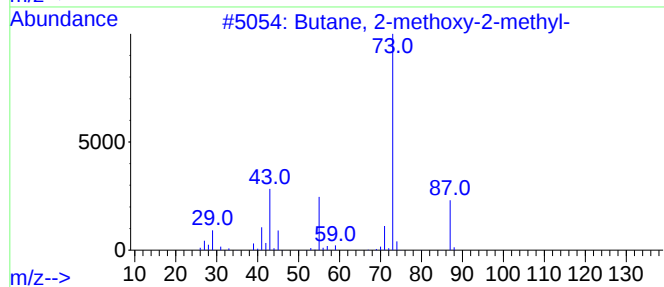
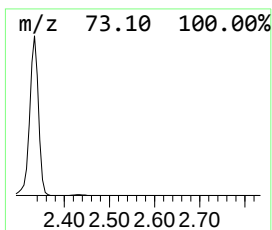
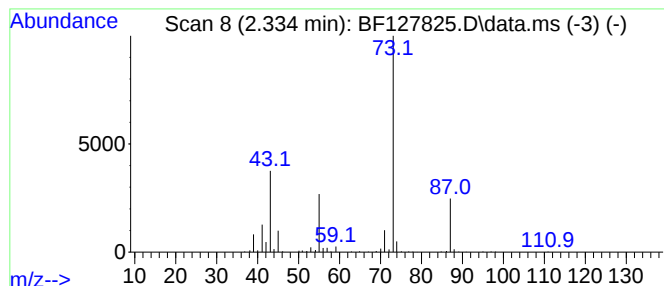
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.334	5.22 ng	254430	1,4-Dichlorobenzene-d4	6.951

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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	32
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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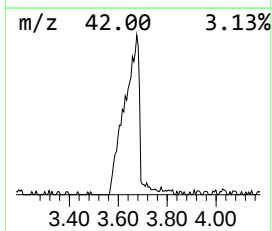
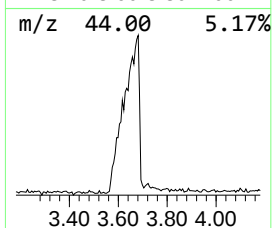
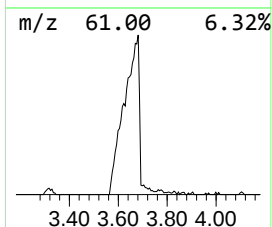
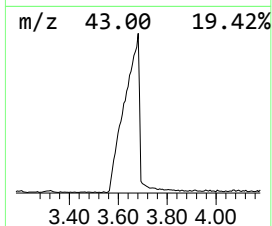
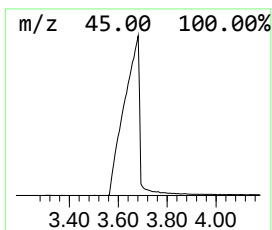
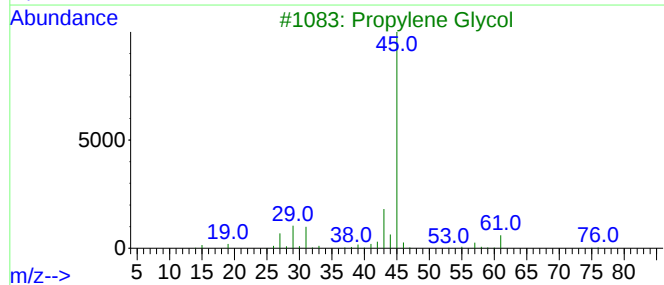
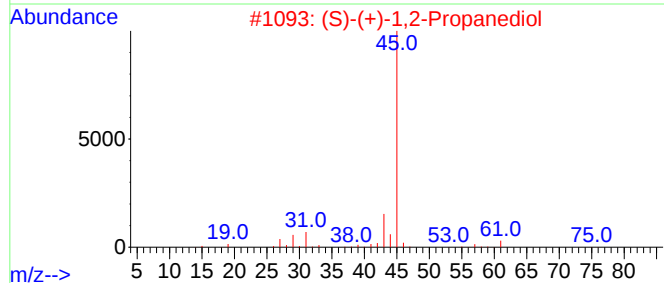
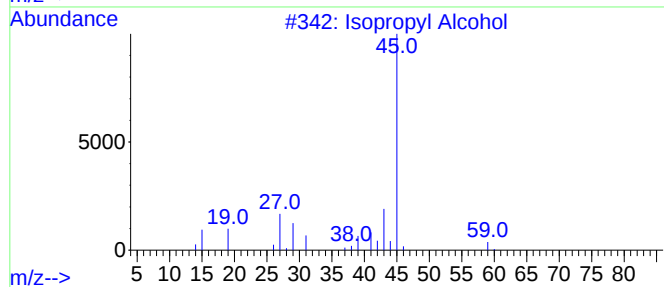
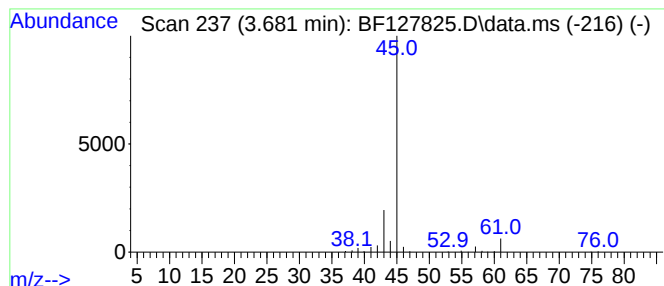
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.681	35.03 ng	1706060	1,4-Dichlorobenzene-d4	6.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3			Propylene Glycol	76	C3H8O2	000057-55-6	43
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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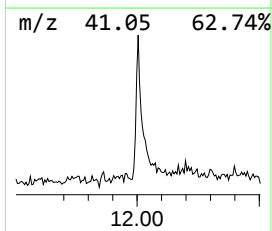
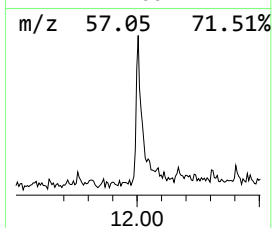
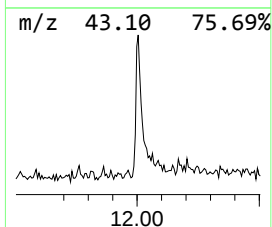
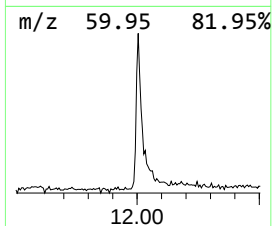
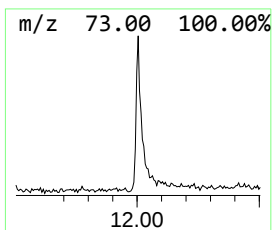
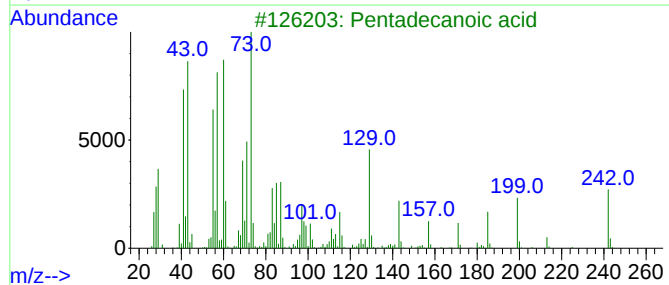
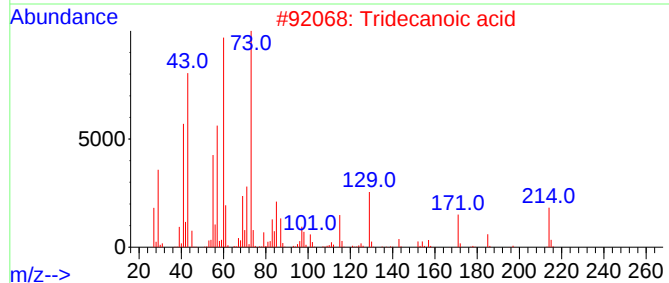
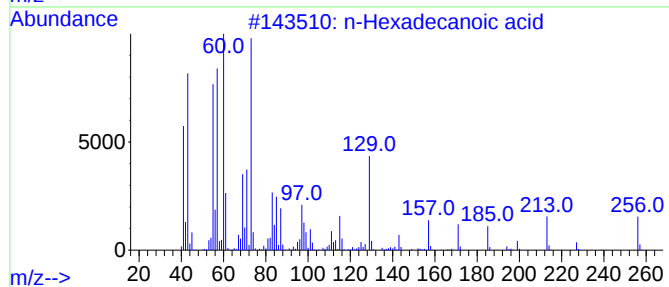
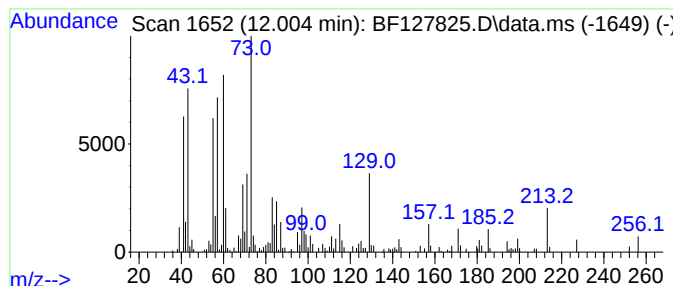
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	2.06 ng	168541	Phenanthrene-d10	11.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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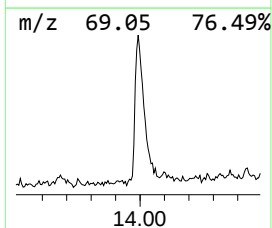
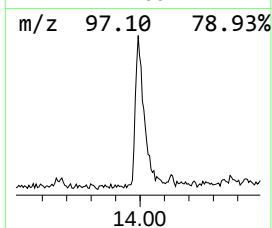
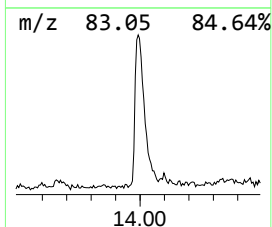
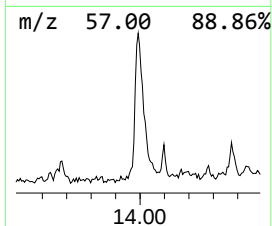
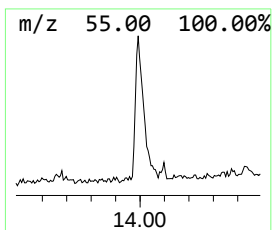
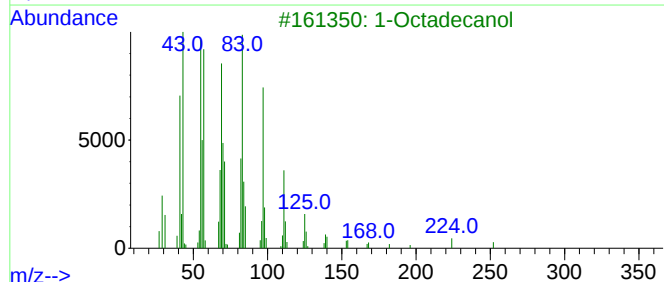
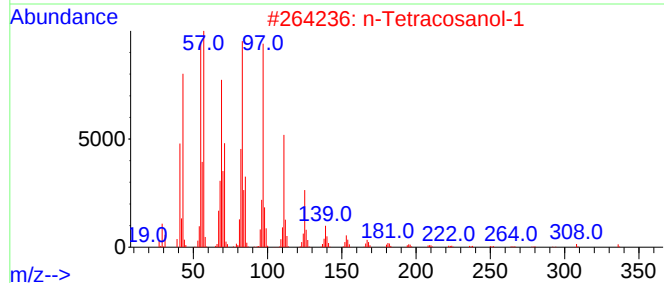
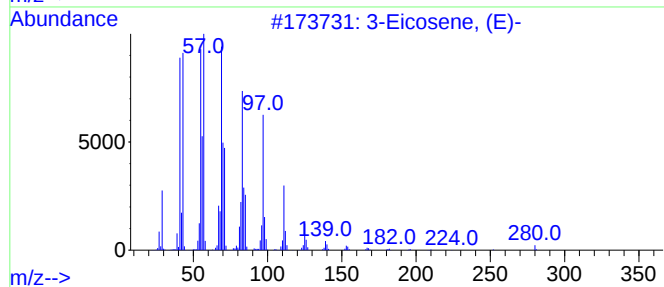
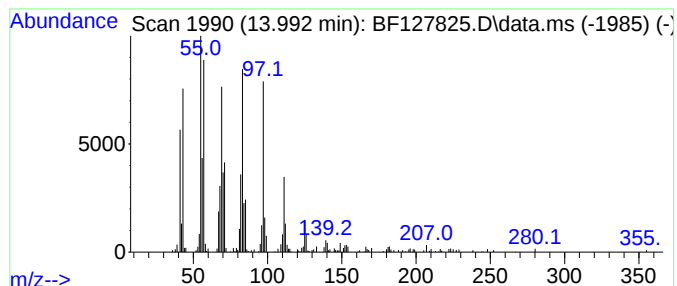
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Peak Number 4 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	8.33 ng	485515	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			1-Octadecanol	270	C18H38O	000112-92-5	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93



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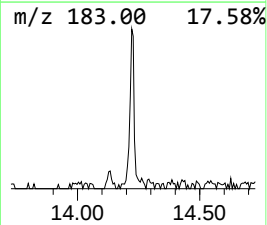
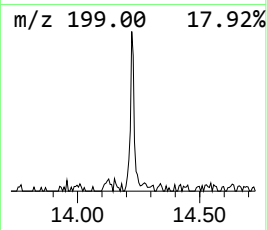
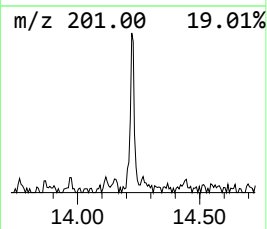
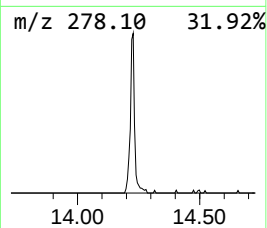
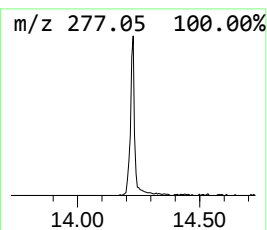
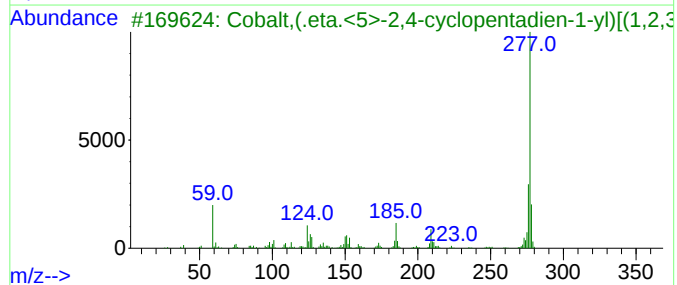
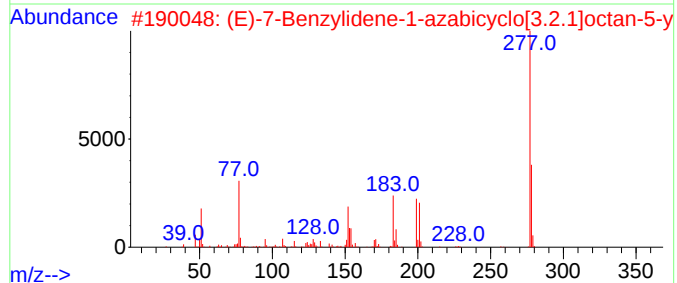
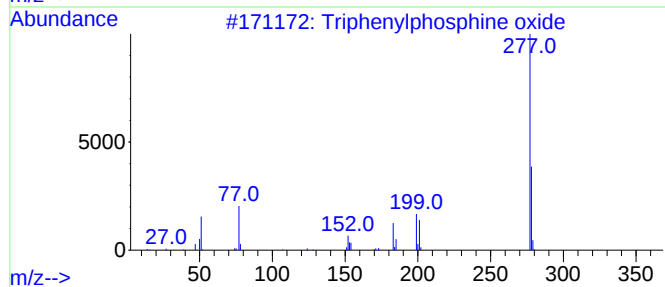
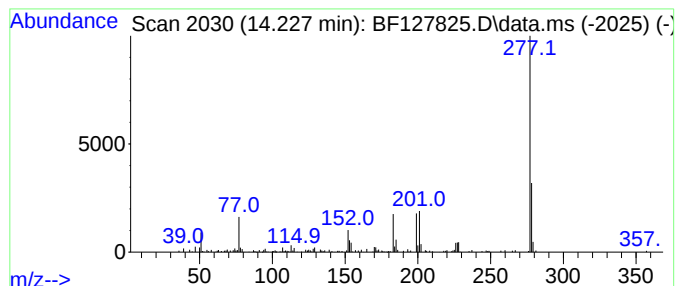
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.227	2.25 ng	131253	Chrysene-d12	14.127

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	43
3			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
4			(Carbathoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	38
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	36



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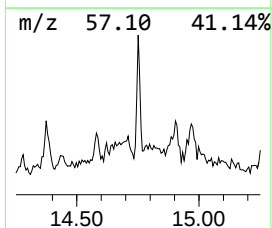
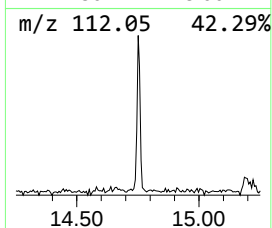
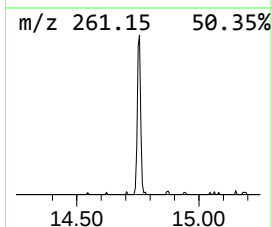
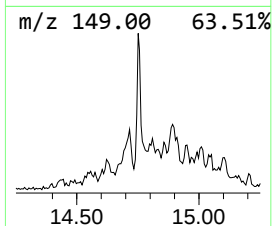
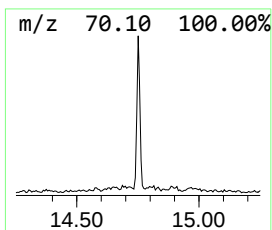
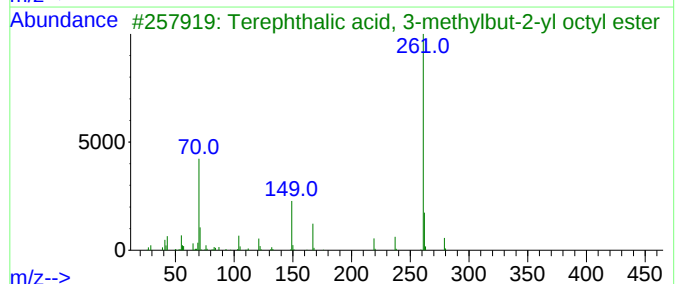
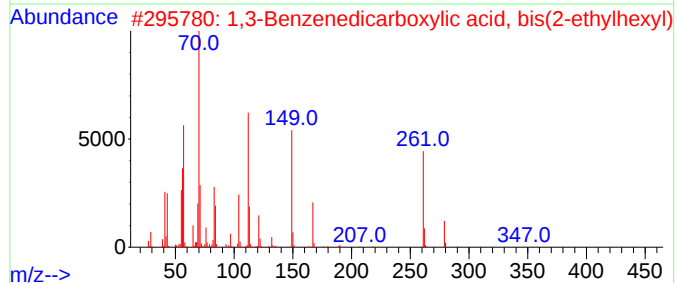
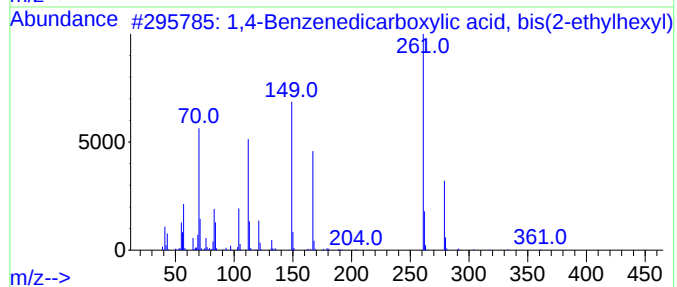
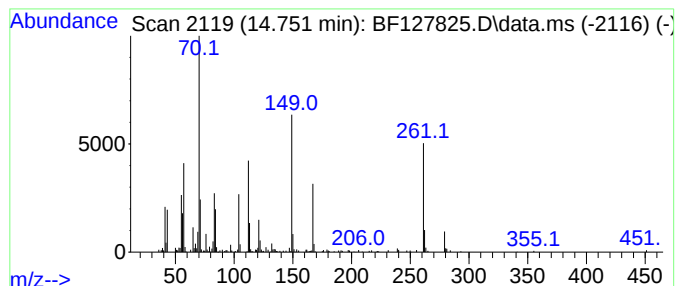
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.751	2.68 ng	156072	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
3			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	53
4			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43
5			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041822\
Data File : BF127825.D
Acq On : 18 Apr 2022 15:12
Operator : CG\JU
Sample : N2442-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.334	5.2	ng	254430	1	6.951	974086	20.0
Isopropyl Alcohol	3.681	35.0	ng	1706060	1	6.951	974086	20.0
n-Hexadecanoic ...	12.004	2.1	ng	168541	4	11.486	1633470	20.0
3-Eicosene, (E)-	13.992	8.3	ng	485515	5	14.127	1165680	20.0
Triphenylphosph...	14.227	2.3	ng	131253	5	14.127	1165680	20.0
1,4-Benzenedica...	14.751	2.7	ng	156072	5	14.127	1165680	20.0