

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120120\
 Data File : BF122522.D
 Acq On : 1 Dec 2020 15:07
 Operator : JU/CG
 Sample : L4906-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 4-DRUM

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-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122522.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	5	7	23	rVB	185251	477582	10.27%	1.356%
2	2.234	23	25	42	rVB	74544	173740	3.74%	0.493%
3	5.069	504	507	516	rVB	39894	52232	1.12%	0.148%
4	5.475	572	576	580	rBV	3188280	3249170	69.90%	9.226%
5	6.486	743	748	767	rBV	3475973	3392683	72.99%	9.634%
6	6.686	779	782	793	rBV	39473	92353	1.99%	0.262%
7	6.857	807	811	814	rBV	1334965	1075058	23.13%	3.053%
8	7.416	901	906	909	rBV	2319846	2131616	45.86%	6.053%
9	8.139	1025	1029	1036	rBV	1618484	1392396	29.95%	3.954%
10	9.216	1208	1212	1224	rBV	4354999	4069236	87.54%	11.555%
11	9.333	1228	1232	1239	rVB2	66614	91661	1.97%	0.260%
12	9.610	1276	1279	1288	rVB	420339	378181	8.14%	1.074%
13	9.898	1324	1328	1331	rBV	1910152	1631180	35.09%	4.632%
14	9.927	1331	1333	1342	rVB	90661	89754	1.93%	0.255%
15	10.445	1417	1421	1427	rVB	80461	74560	1.60%	0.212%
16	10.686	1458	1462	1477	rBV	2840822	2756751	59.30%	7.828%
17	11.386	1577	1581	1583	rBV	1811949	1776117	38.21%	5.043%
18	11.404	1583	1584	1588	rVV	507779	426287	9.17%	1.210%
19	11.457	1591	1593	1597	rVB	119498	106432	2.29%	0.302%
20	11.886	1660	1666	1667	rBV	55556	49386	1.06%	0.140%
21	11.916	1667	1671	1677	rVV2	301895	340806	7.33%	0.968%
22	11.998	1682	1685	1688	rBV	94364	95797	2.06%	0.272%
23	12.598	1784	1787	1793	rBV	770701	633953	13.64%	1.800%
24	12.698	1800	1804	1811	rBV	328141	461175	9.92%	1.310%
25	12.827	1818	1826	1828	rBV	568489	612098	13.17%	1.738%
26	12.974	1846	1851	1854	rBV	5052219	4648454	100.00%	13.200%
27	13.157	1875	1882	1885	rVB	104614	139659	3.00%	0.397%
28	13.221	1885	1893	1896	rBV	114109	123191	2.65%	0.350%
29	13.257	1896	1899	1902	rBV2	49121	49470	1.06%	0.140%
30	13.945	2010	2016	2023	rBV3	114197	306436	6.59%	0.870%
31	14.027	2024	2030	2033	rVV	1927614	2058759	44.29%	5.846%
32	14.051	2033	2034	2037	rVB	144604	76029	1.64%	0.216%
33	14.498	2105	2110	2114	rBV4	51326	82683	1.78%	0.235%
34	15.068	2203	2207	2216	rBV	115116	225118	4.84%	0.639%
35	15.145	2217	2220	2223	rVB	56672	57356	1.23%	0.163%
36	15.368	2255	2258	2264	rVB	55767	78879	1.70%	0.224%

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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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.433	2265	2269	2275	rVV	83290	104598	2.25%	0.297%
38	15.498	2275	2280	2294	rVB	1136533	1574208	33.87%	4.470%
39	15.968	2355	2360	2366	rVB2	36682	61213	1.32%	0.174%

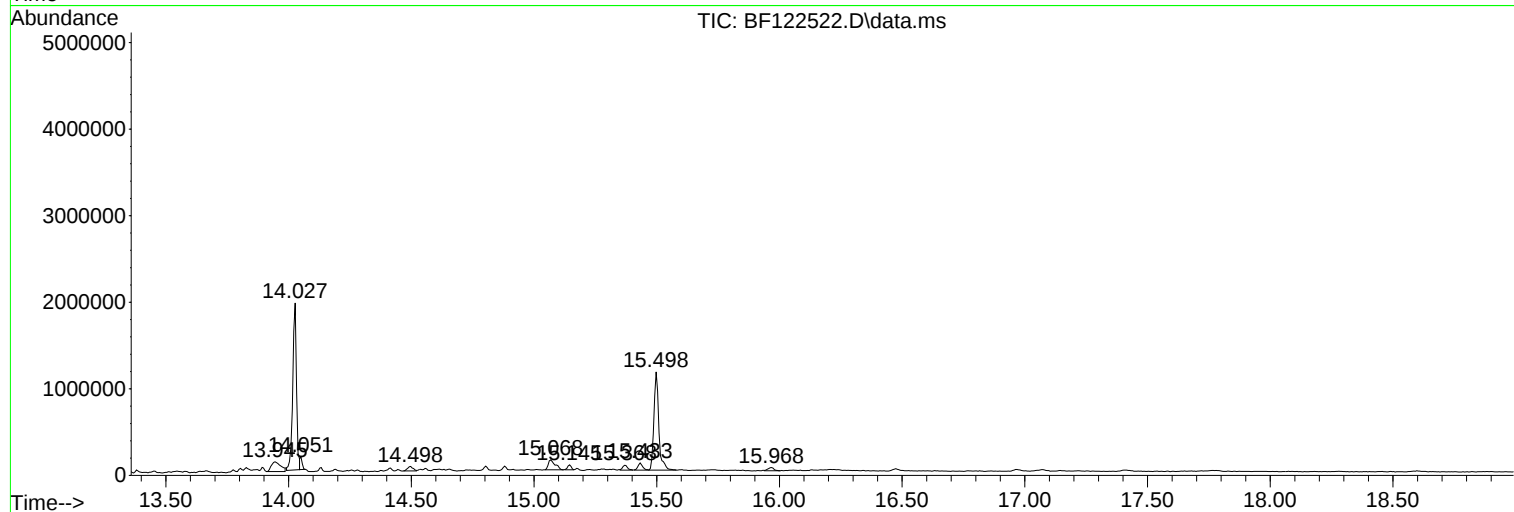
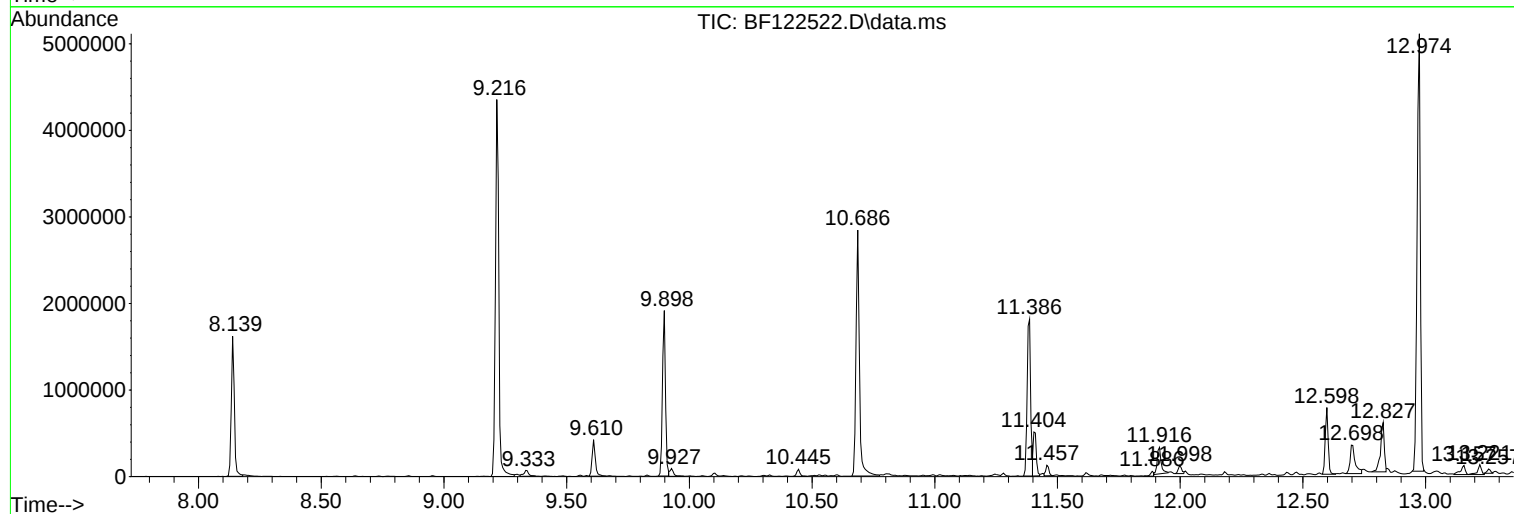
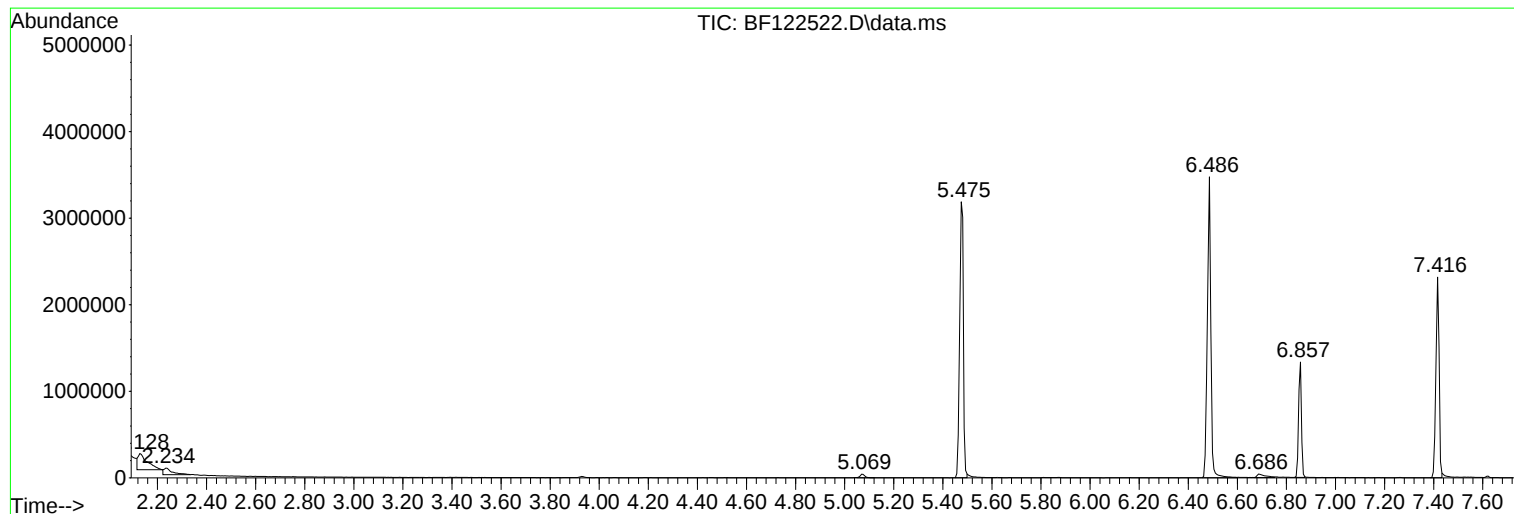
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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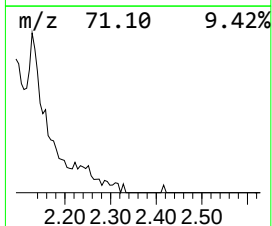
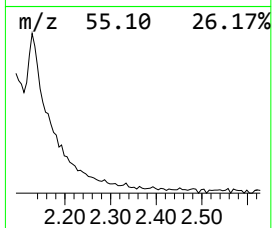
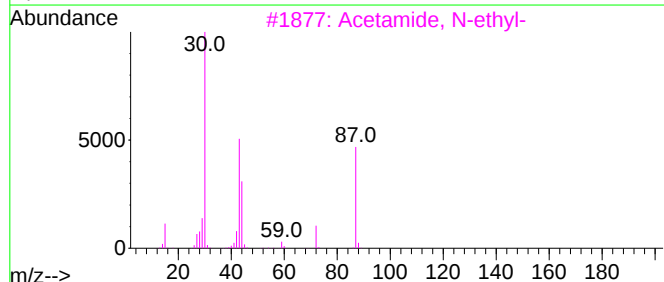
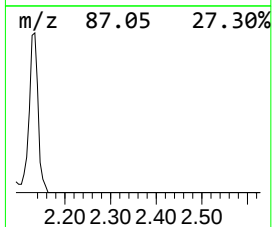
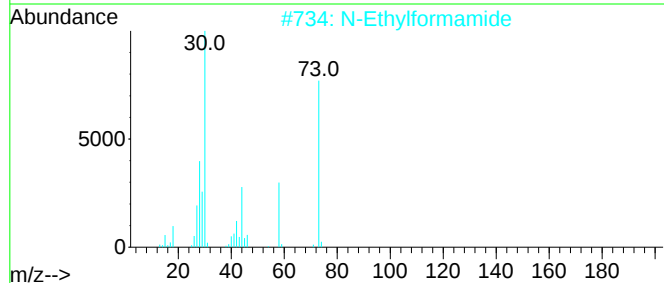
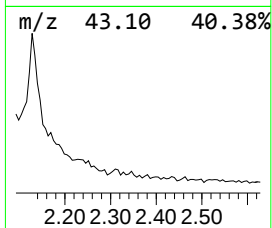
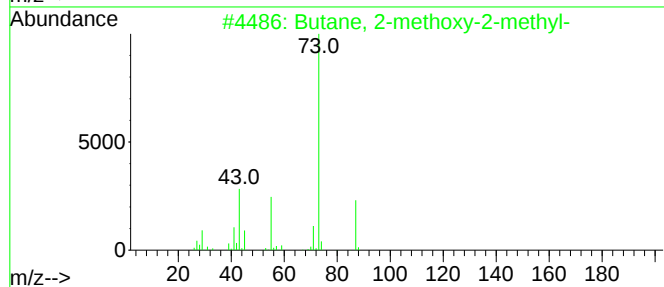
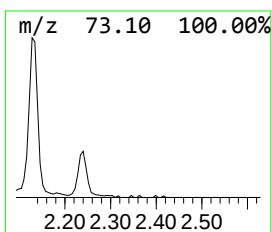
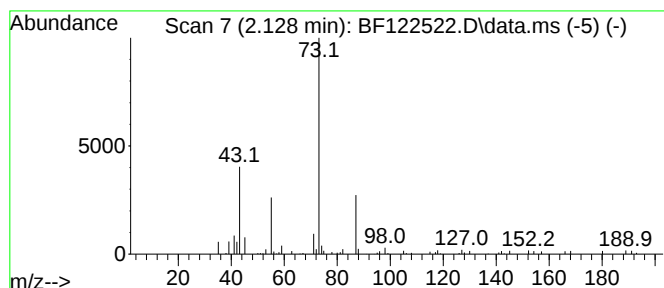
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	8.88 ng	477582	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2			N-Ethylformamide	73	C3H7NO	000627-45-2	9
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4			2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	9
5			Hexane, 2,5-dimethoxy-2,5-dimethyl-	174	C10H22O2	053273-13-5	9



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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4-DRUM

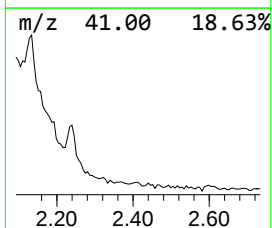
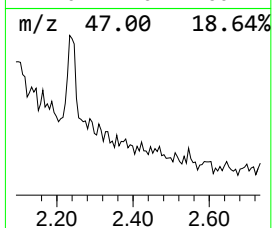
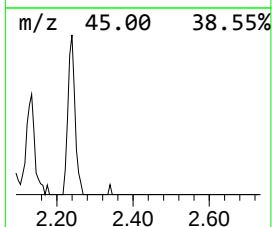
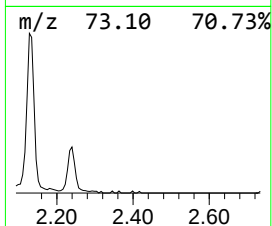
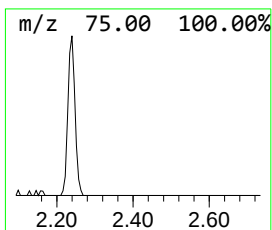
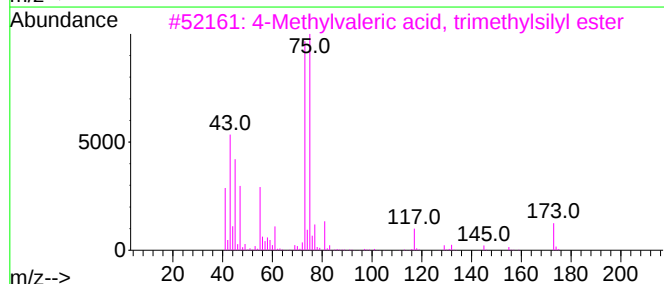
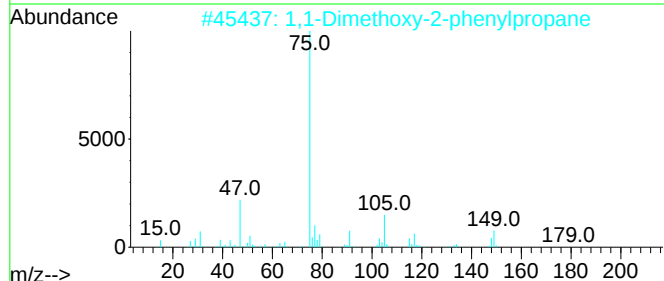
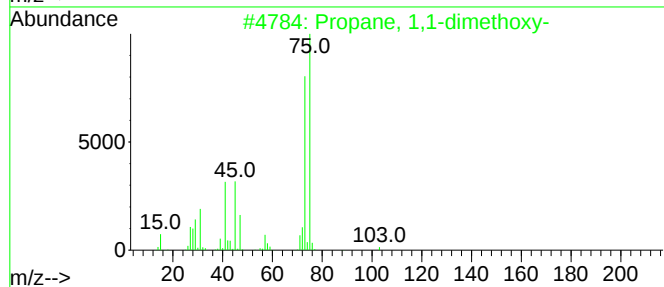
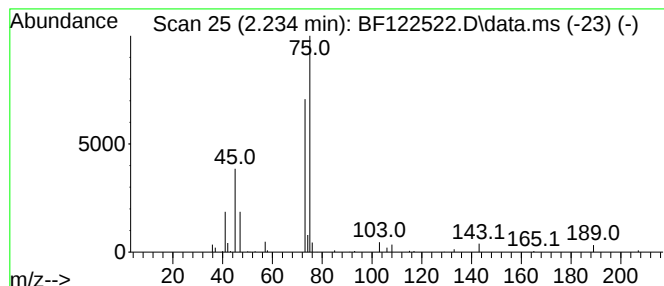
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	3.23 ng	173740	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			1,1-Dimethoxy-2-phenylpropane	180	C11H16O2	000090-87-9	28
3			4-Methylvaleric acid, trimethylsilyl ester	188	C9H20O2Si	959048-10-3	28
4			Ethanethiol, 2-trimethylsiloxy-	150	C5H14OSSi	037515-85-8	9
5			Benzene, [2-(ethylthio)ethyl]-	166	C10H14S	022914-08-5	9



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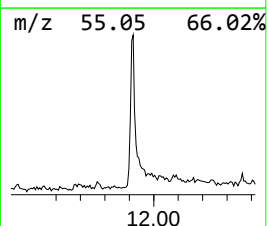
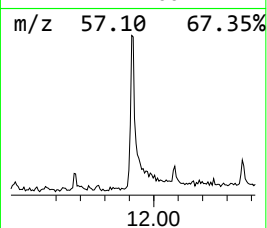
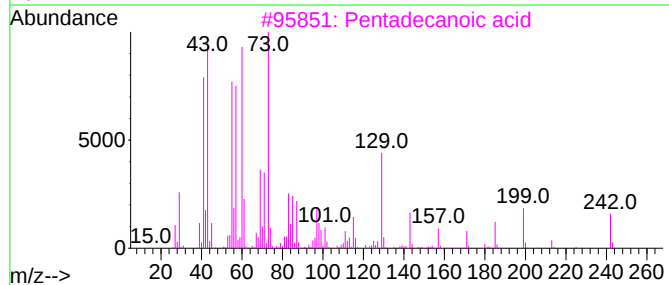
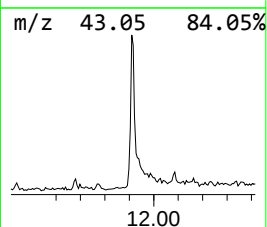
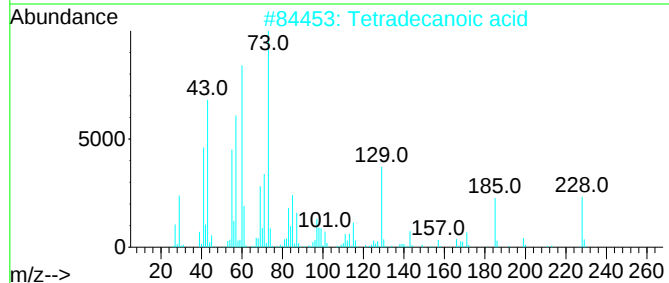
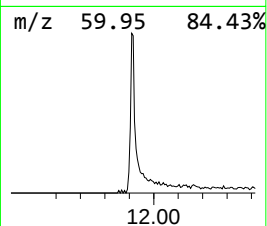
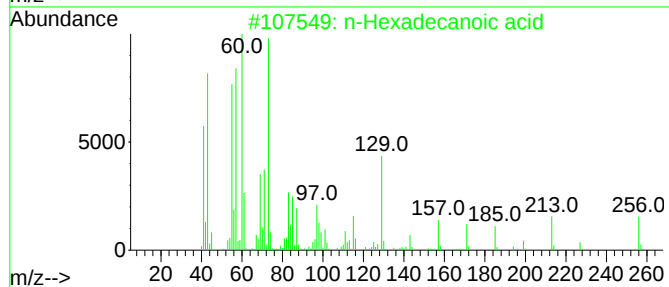
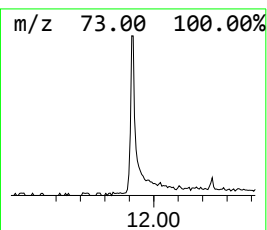
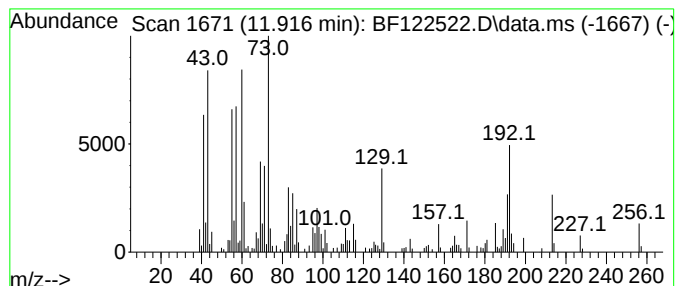
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.84 ng	340806	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tridecanoic acid	214	C13H26O2	000638-53-9	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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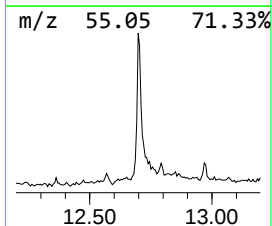
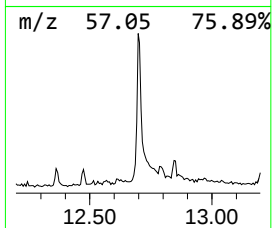
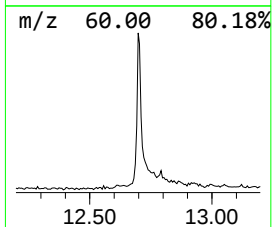
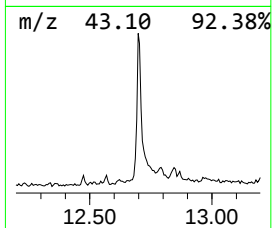
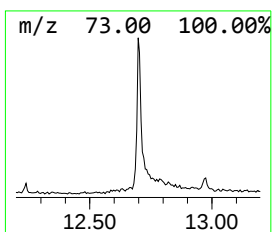
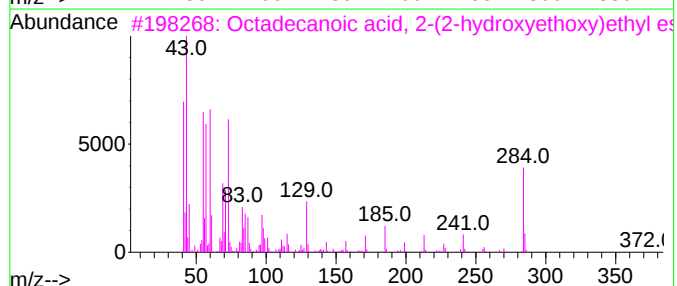
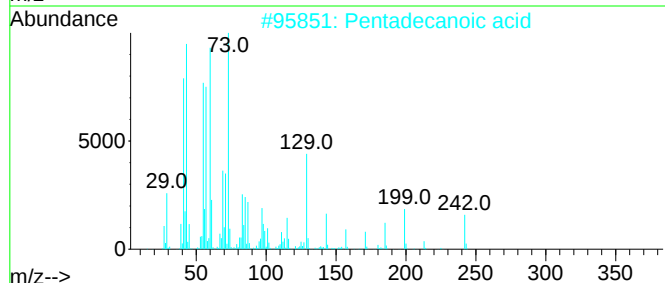
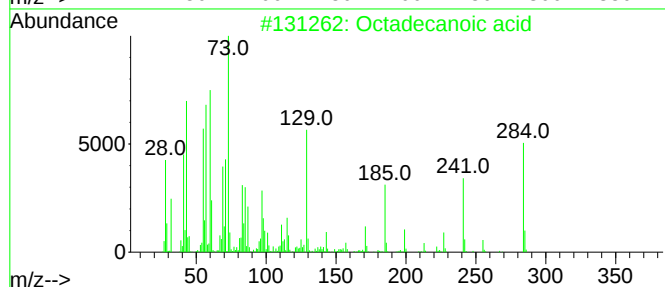
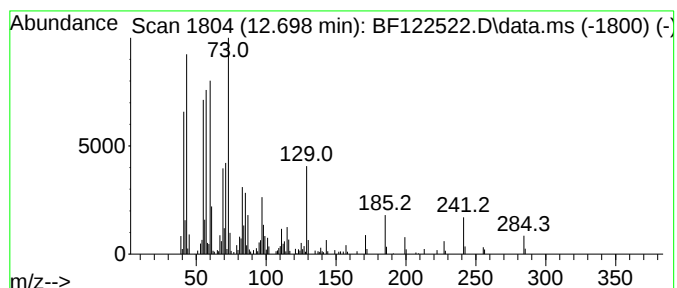
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	5.19 ng	461175	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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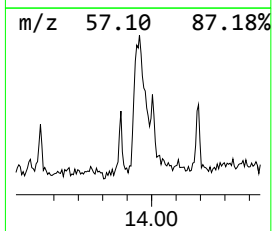
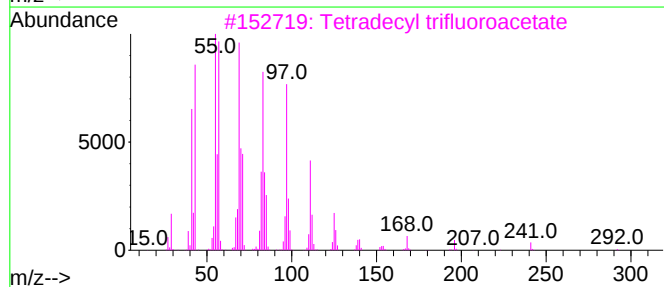
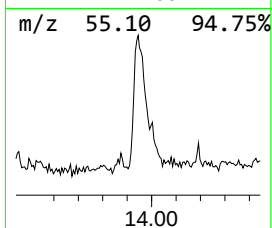
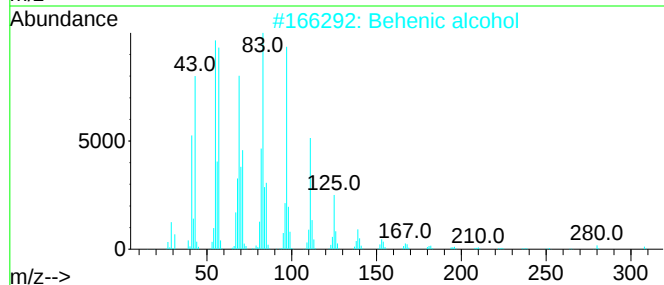
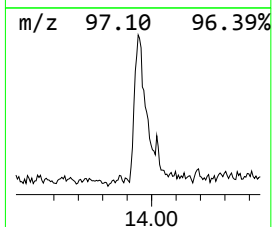
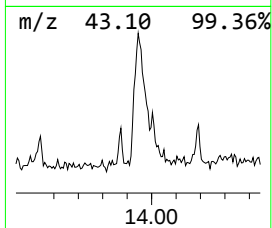
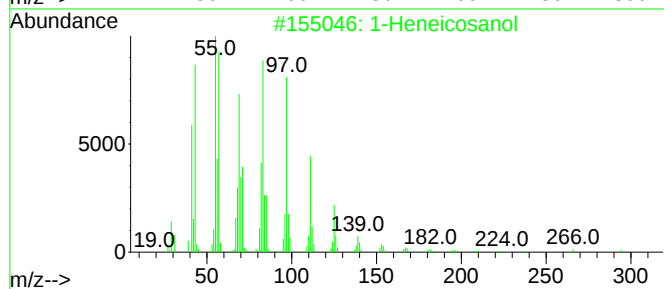
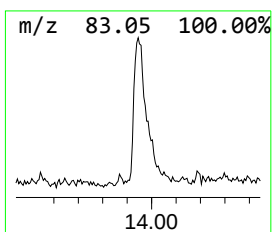
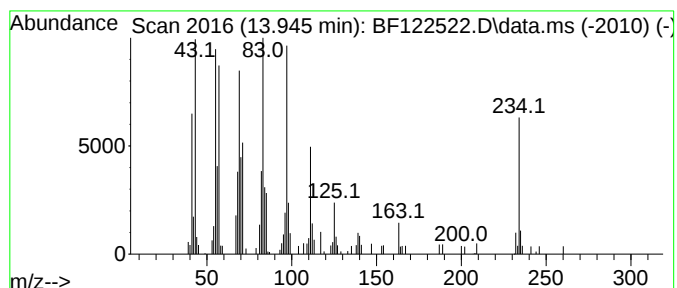
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	2.98 ng	306436	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	93
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120120\
Data File : BF122522.D
Acq On : 1 Dec 2020 15:07
Operator : JU/CG
Sample : L4906-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.12	2.128	8.9	ng	477582	1	6.857	1075060	20.0
Propane, 1,1-di...	2.234	3.2	ng	173740	1	6.857	1075060	20.0
n-Hexadecanoic ...	11.916	3.8	ng	340806	4	11.386	1776120	20.0
Octadecanoic acid	12.698	5.2	ng	461175	4	11.386	1776120	20.0
1-Heneicosanol	13.945	3.0	ng	306436	5	14.027	2058760	20.0