

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
 Data File : BF125241.D
 Acq On : 27 Aug 2021 00:03
 Operator : JU/CG
 Sample : M3547-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-1

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125241.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	18	29	35	rVB	1476080	2096181	37.26%	4.016%
2	4.040	328	332	337	rVB	56931	68543	1.22%	0.131%
3	5.151	511	521	526	rBV	86542	114828	2.04%	0.220%
4	5.540	582	587	590	rBV	4925603	4805188	85.40%	9.207%
5	6.539	751	757	760	rBV	4577122	4710753	83.72%	9.026%
6	6.910	817	820	824	rBV	1464644	1263234	22.45%	2.420%
7	7.475	911	916	919	rBV	3355828	3120675	55.46%	5.979%
8	8.092	1018	1021	1032	rBV	138161	286502	5.09%	0.549%
9	8.192	1035	1038	1042	rVB	1699055	1584092	28.15%	3.035%
10	8.780	1135	1138	1141	rVB	101249	79500	1.41%	0.152%
11	9.269	1216	1221	1224	rBV	6204003	5424546	96.41%	10.393%
12	9.345	1230	1234	1237	rBV	150736	125653	2.23%	0.241%
13	9.875	1320	1324	1328	rVB	188566	154203	2.74%	0.295%
14	9.951	1333	1337	1340	rVV	1916937	1700431	30.22%	3.258%
15	10.374	1406	1409	1412	rVB	199104	162179	2.88%	0.311%
16	10.592	1442	1446	1453	rVB	72384	87720	1.56%	0.168%
17	10.739	1464	1471	1474	rBV	3717032	3313341	58.89%	6.348%
18	10.845	1486	1489	1494	rBV2	221389	282121	5.01%	0.541%
19	11.292	1562	1565	1568	rBV	188847	153685	2.73%	0.294%
20	11.321	1568	1570	1577	rVB3	88421	97713	1.74%	0.187%
21	11.433	1586	1589	1592	rBV	1711807	1643244	29.21%	3.148%
22	11.721	1635	1638	1641	rBV	173631	133028	2.36%	0.255%
23	11.810	1649	1653	1656	rBV	6480989	5626529	100.00%	10.780%
24	11.951	1673	1677	1686	rBV3	401611	417147	7.41%	0.799%
25	12.127	1704	1707	1711	rBV	138812	107706	1.91%	0.206%
26	12.498	1766	1770	1777	rBV	5852114	5445051	96.77%	10.433%
27	12.651	1793	1796	1805	rVB	124626	135967	2.42%	0.261%
28	12.739	1807	1811	1819	rBV2	130446	160826	2.86%	0.308%
29	12.880	1829	1835	1839	rBV2	128611	173628	3.09%	0.333%
30	13.021	1854	1859	1862	rBV	5447487	5165029	91.80%	9.896%
31	13.968	2013	2020	2023	rBV5	111897	291043	5.17%	0.558%
32	14.074	2034	2038	2041	rBV	1567666	1370667	24.36%	2.626%
33	14.833	2164	2167	2174	rVB2	70736	109849	1.95%	0.210%
34	15.004	2193	2196	2199	rVB2	80873	79570	1.41%	0.152%
35	15.127	2214	2217	2225	rVV	59874	112060	1.99%	0.215%
36	15.198	2227	2229	2233	rVB	68733	68387	1.22%	0.131%

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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PE-1

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-BF081821.M
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37	15.574	2287	2293	2302	rBV	982724	1406891	25.00%	2.696%
38	16.045	2369	2373	2379	rVB	70969	114281	2.03%	0.219%

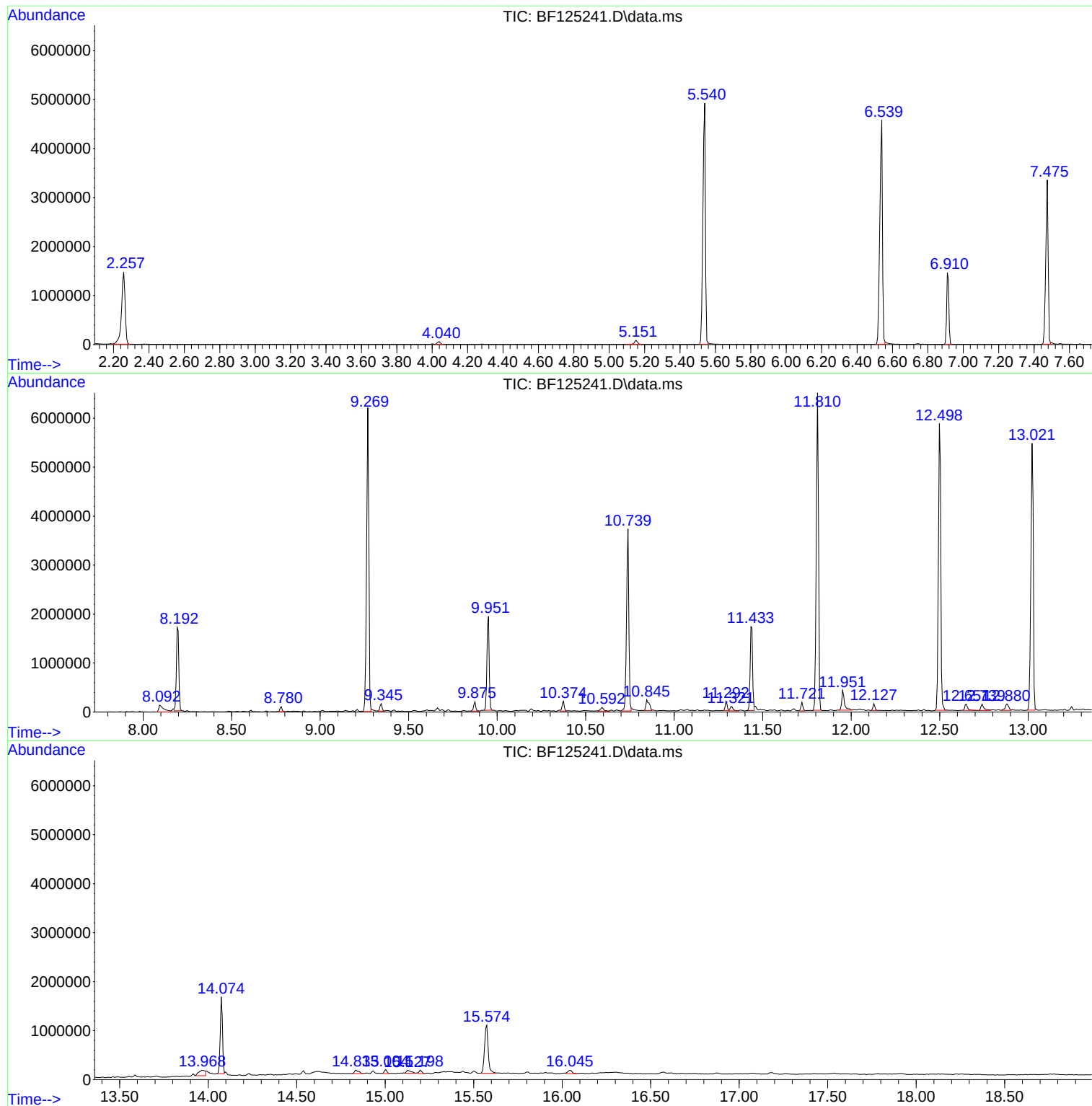
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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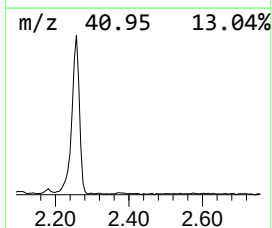
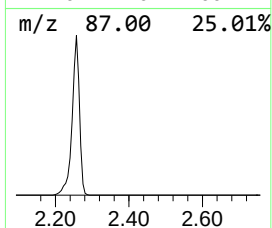
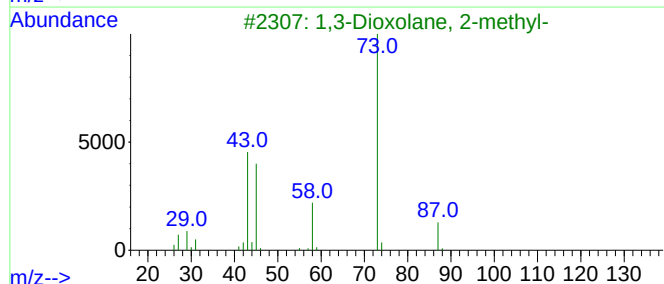
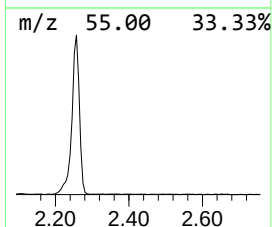
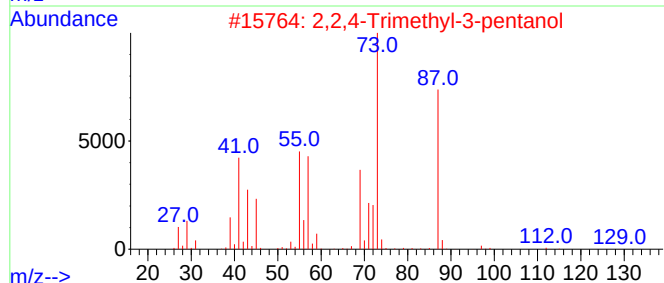
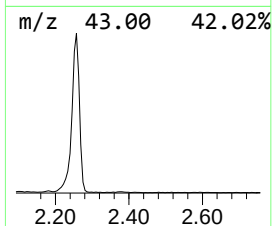
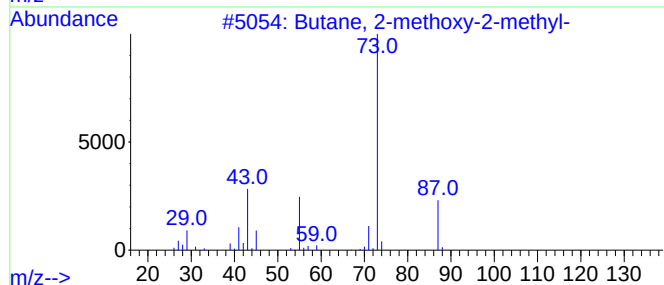
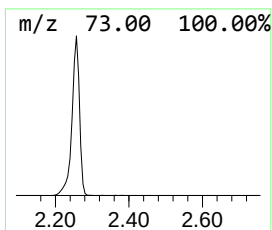
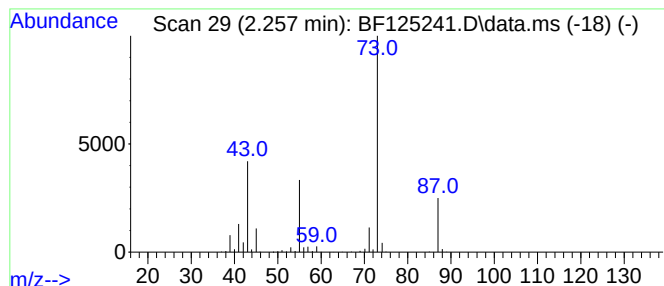
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	33.19 ng	2096180	1,4-Dichlorobenzene-d4	6.916

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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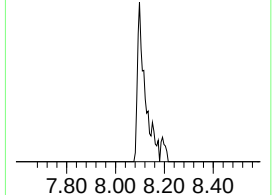
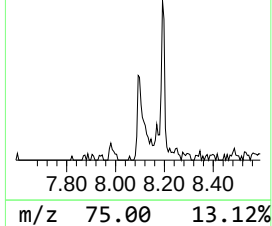
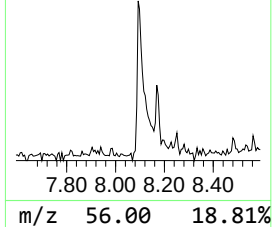
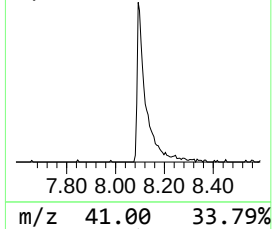
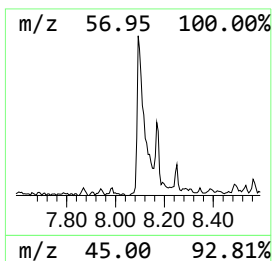
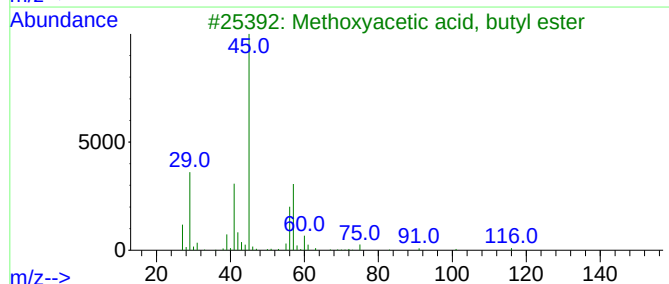
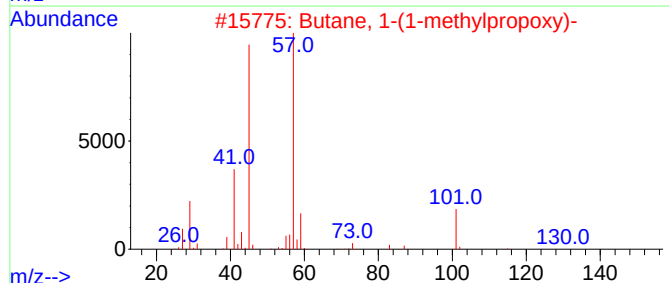
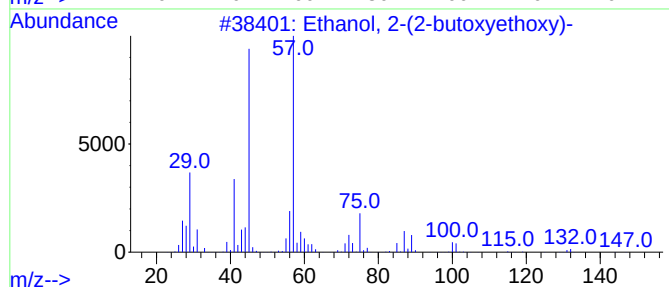
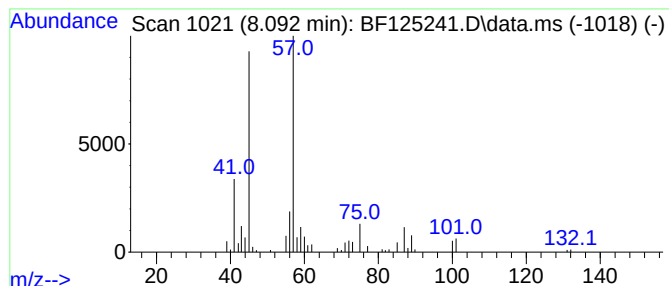
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	3.62 ng	286502	Naphthalene-d8	8.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
3			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	53
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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Instrument :
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ClientSampled :
PE-1

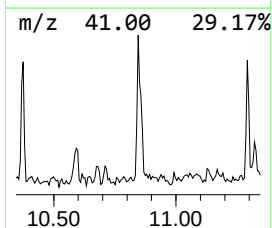
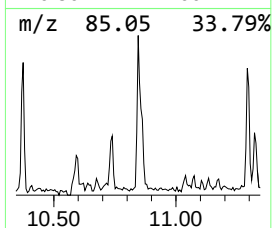
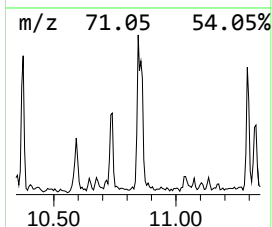
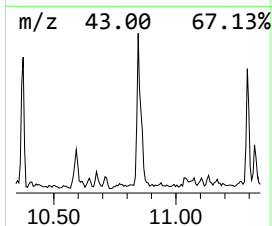
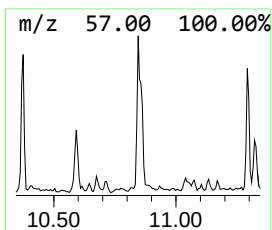
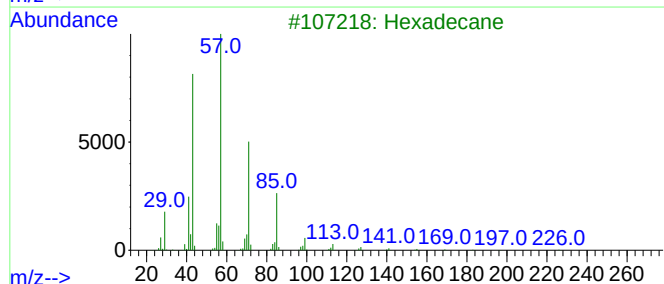
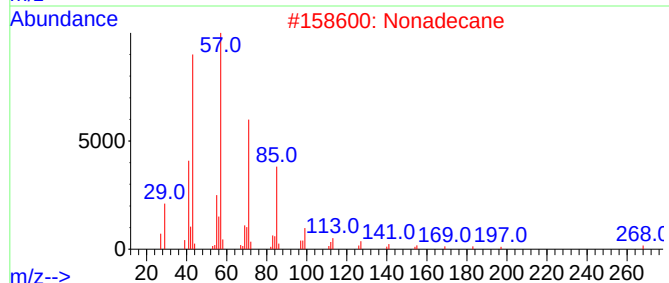
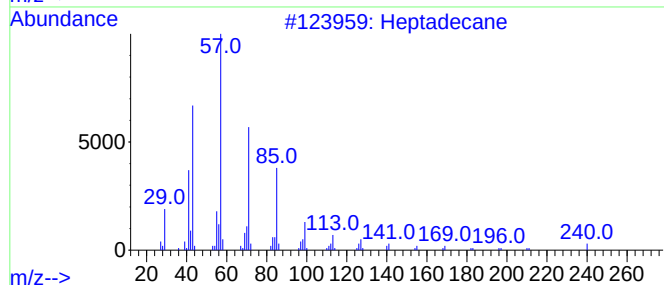
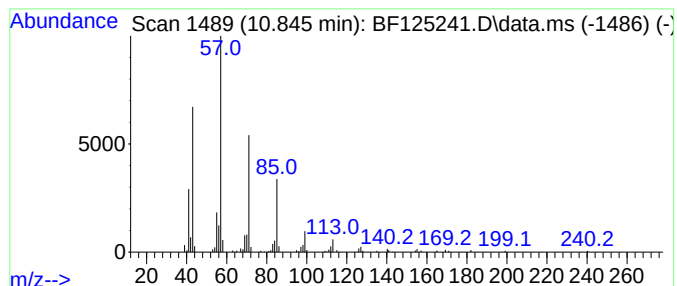
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.845	3.43 ng	282121	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	97
2			Nonadecane	268	C19H40	000629-92-5	87
3			Hexadecane	226	C16H34	000544-76-3	86
4			Tridecane	184	C13H28	000629-50-5	86
5			Tetradecane	198	C14H30	000629-59-4	86



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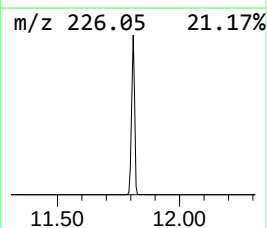
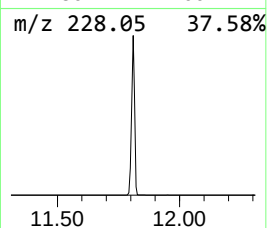
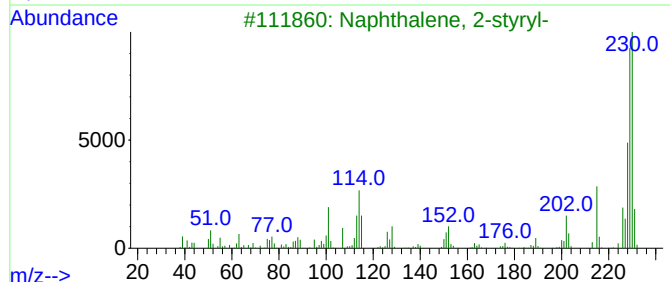
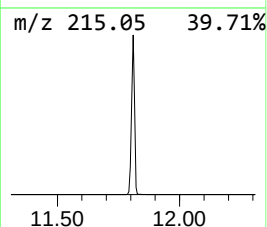
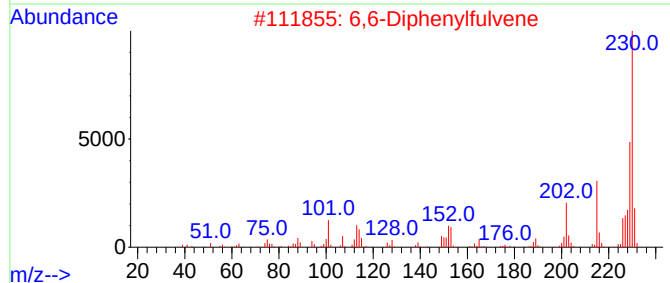
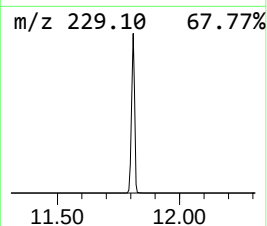
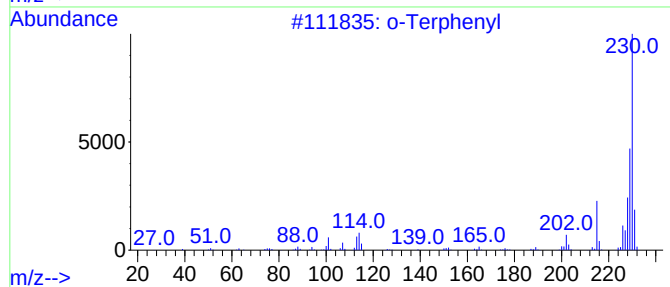
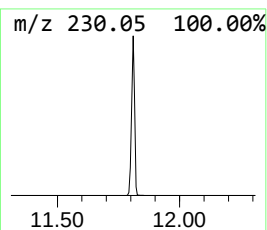
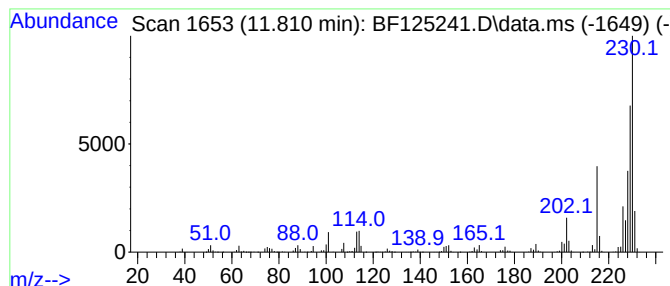
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 o-Terphenyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	68.48 ng	5626530	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Terphenyl	230	C18H14	000084-15-1	97
2			6,6-Diphenylfulvene	230	C18H14	002175-90-8	91
3			Naphthalene, 2-styryl-	230	C18H14	002039-70-5	86
4			Pyrene, 1,3-dimethyl-	230	C18H14	064401-21-4	83
5			Benz[a]anthracene, 7,12-dihydro-	230	C18H14	016434-59-6	49



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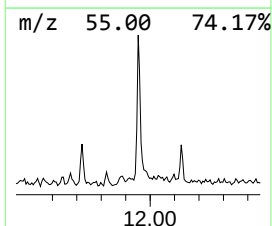
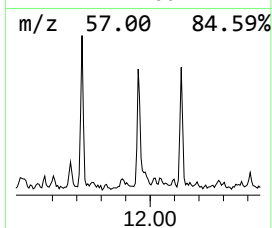
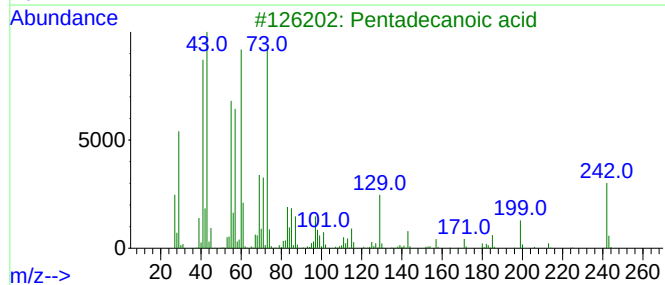
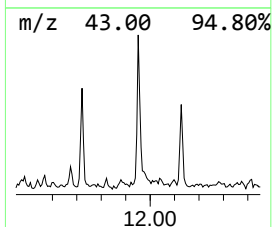
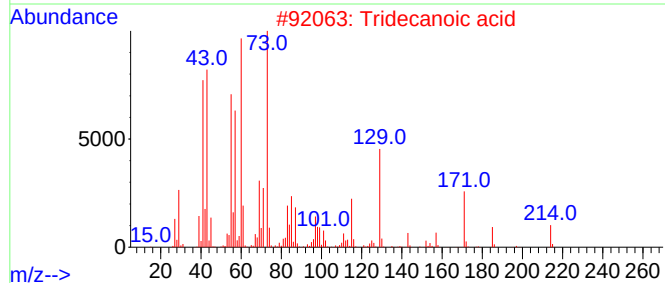
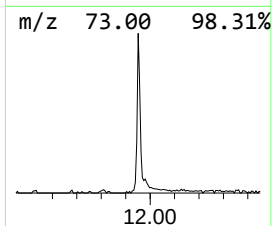
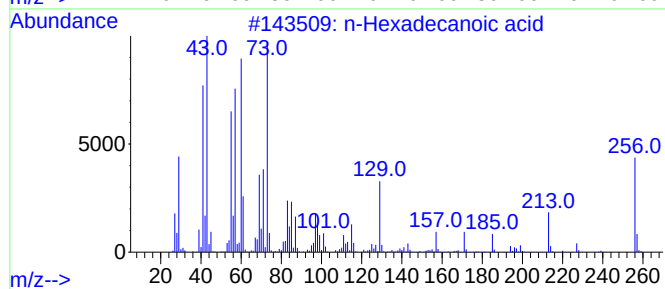
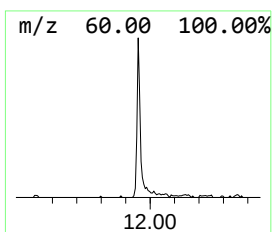
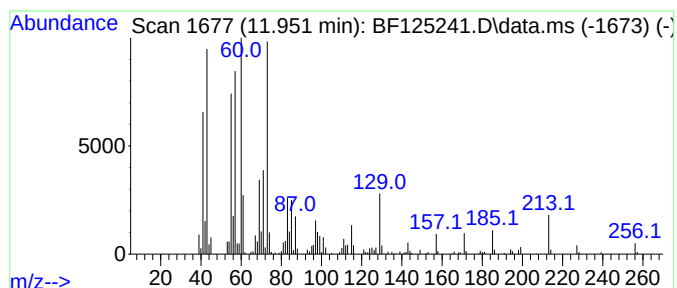
Instrument :
BNA_F
ClientSampleId :
PE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.951	5.08 ng	417147	Phenanthrene-d10	11.439	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
Data File : BF125241.D
Acq On : 27 Aug 2021 00:03
Operator : JU/CG
Sample : M3547-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

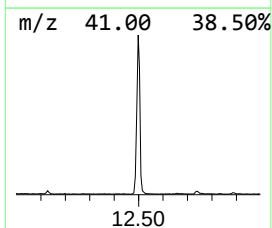
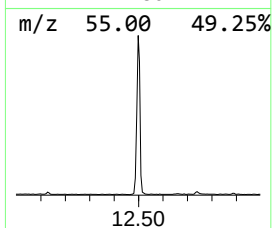
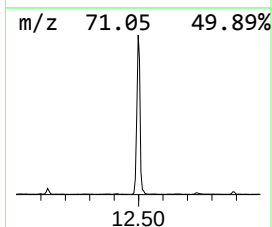
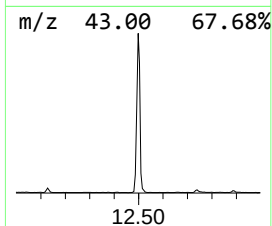
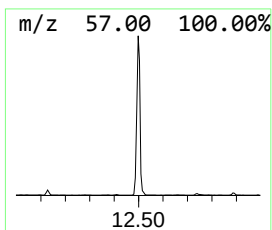
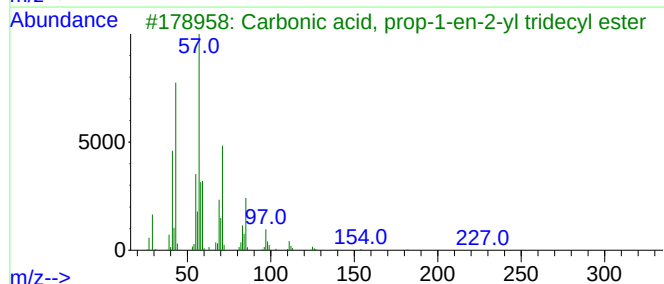
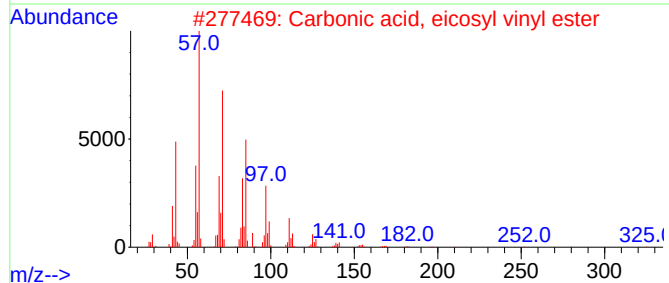
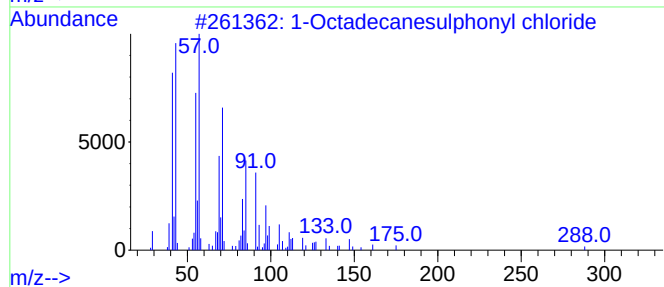
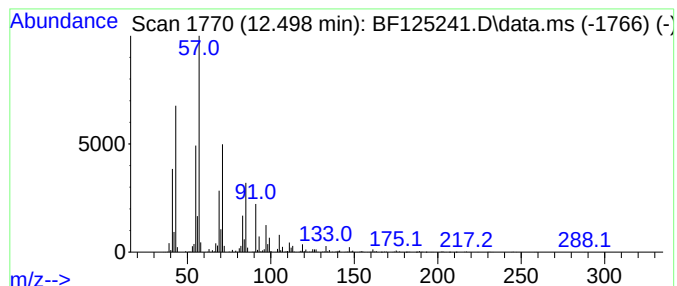
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Octadecanesulphonyl chloride Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.498	66.27 ng	5445050	Phenanthrene-d10		11.439	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride		352	C18H37ClO2S	1000342-70-4	91
2	Carbonic acid, eicosyl vinyl ester		368	C23H44O3	1000382-54-3	90
3	Carbonic acid, prop-1-en-2-yl tr...		284	C17H32O3	1000382-90-8	83
4	Octadecane, 1-chloro-		288	C18H37Cl	003386-33-2	78
5	Nonadecane		268	C19H40	000629-92-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082621\
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Acq On : 27 Aug 2021 00:03
Operator : JU/CG
Sample : M3547-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-1

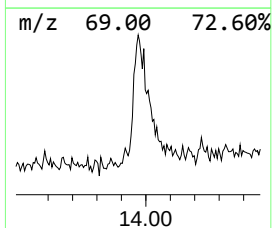
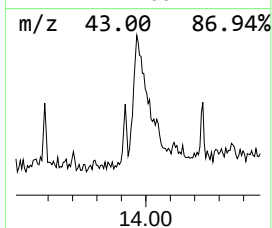
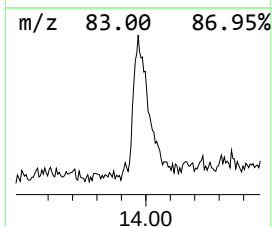
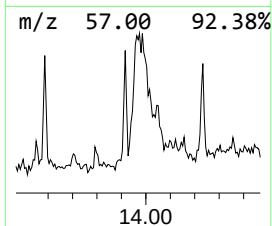
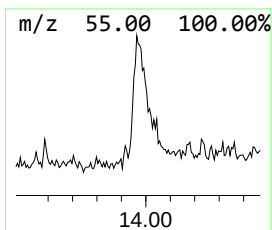
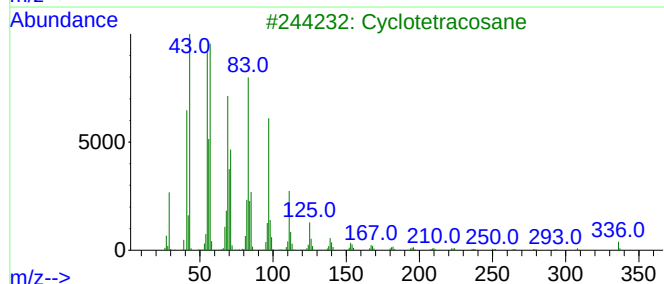
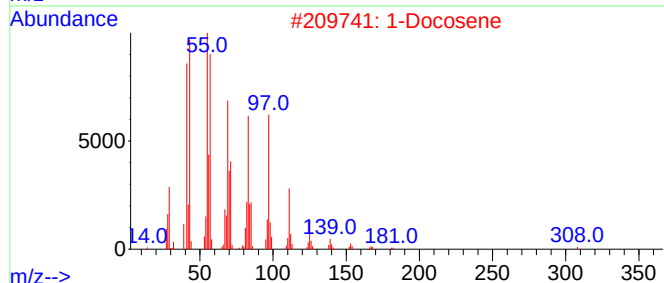
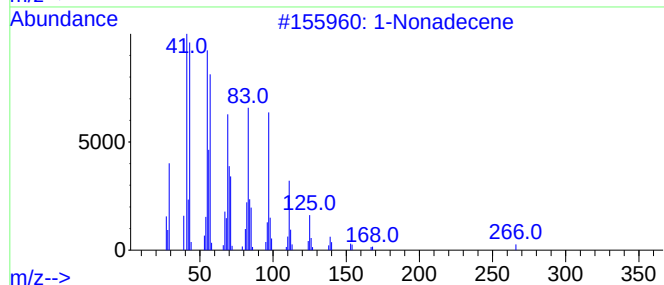
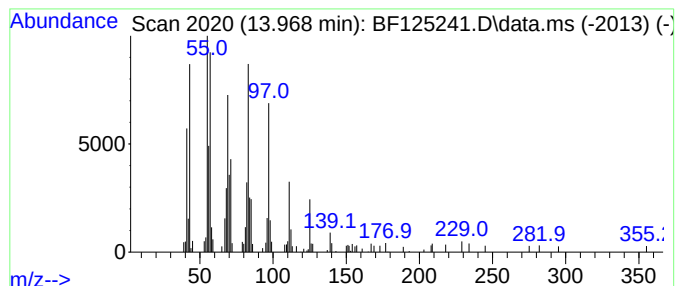
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.968	4.25 ng	291043	Chrysene-d12	14.074

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	91
2	1-Docosene		308	C22H44	001599-67-3	91
3	Cyclotetracosane		336	C24H48	000297-03-0	91
4	1-Heneicosanol		312	C21H44O	015594-90-8	91
5	10-Heneicosene (c,t)		294	C21H42	095008-11-0	91



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Sample : M3547-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.257	33.2	ng	2096180	1	6.916	1263230	20.0
Ethanol, 2-(2-b...	8.092	3.6	ng	286502	2	8.192	1584090	20.0
Heptadecane	10.845	3.4	ng	282121	4	11.439	1643240	20.0
o-Terphenyl	11.810	68.5	ng	5626530	4	11.439	1643240	20.0
n-Hexadecanoic ...	11.951	5.1	ng	417147	4	11.439	1643240	20.0
1-Octadecanesul...	12.498	66.3	ng	5445050	4	11.439	1643240	20.0
1-Nonadecene	13.968	4.3	ng	291043	5	14.074	1370670	20.0