

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083121\
 Data File : BF125284.D
 Acq On : 31 Aug 2021 12:32
 Operator : JU/CG
 Sample : M3561-19
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EB-082621

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: BF125284.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	12	18	24	rVB	3272632	4174025	55.68%	10.663%
2	5.528	581	585	600	rBV	937748	894306	11.93%	2.285%
3	6.534	753	756	773	rVB	633939	615794	8.21%	1.573%
4	6.910	817	820	824	rBV	1364004	1140629	15.21%	2.914%
5	7.481	911	917	920	rBV	3195697	3227771	43.05%	8.246%
6	8.098	1018	1022	1035	rBV	968646	1329832	17.74%	3.397%
7	8.198	1035	1039	1042	rVV	1708378	1496376	19.96%	3.823%
8	9.269	1216	1221	1225	rBV	5743390	5655645	75.44%	14.448%
9	9.381	1237	1240	1245	rBV	177764	170148	2.27%	0.435%
10	9.533	1263	1266	1272	rBV2	98341	113541	1.51%	0.290%
11	9.604	1272	1278	1281	rVV2	61800	79690	1.06%	0.204%
12	9.663	1285	1288	1291	rVB2	83341	79734	1.06%	0.204%
13	9.951	1332	1337	1345	rVB	2092463	1816573	24.23%	4.641%
14	10.592	1442	1446	1451	rVB	89477	112987	1.51%	0.289%
15	10.739	1467	1471	1484	rVB	2386387	2217220	29.57%	5.664%
16	10.857	1487	1491	1495	rBV	164378	144620	1.93%	0.369%
17	11.322	1567	1570	1576	rVB3	83505	99517	1.33%	0.254%
18	11.439	1586	1590	1593	rBV	2299836	1967116	26.24%	5.025%
19	11.822	1651	1655	1658	rBV	284774	212946	2.84%	0.544%
20	11.957	1672	1678	1683	rBV2	449012	465056	6.20%	1.188%
21	12.616	1787	1790	1793	rVB	185320	156988	2.09%	0.401%
22	12.739	1808	1811	1818	rBV2	111300	128379	1.71%	0.328%
23	13.027	1855	1860	1863	rBV	6896212	7497061	100.00%	19.152%
24	13.939	2008	2015	2028	rBV2	282656	697665	9.31%	1.782%
25	14.080	2035	2039	2043	rBV	2242408	1997593	26.65%	5.103%
26	14.539	2113	2117	2119	rBV	71465	77551	1.03%	0.198%
27	14.851	2165	2170	2174	rBV2	88239	129578	1.73%	0.331%
28	14.933	2180	2184	2188	rBV	190770	200132	2.67%	0.511%
29	15.204	2226	2230	2237	rBV	79485	101422	1.35%	0.259%
30	15.586	2289	2295	2305	rBV	1353035	1958971	26.13%	5.004%
31	16.045	2369	2373	2379	rVB	66950	98266	1.31%	0.251%
32	16.562	2459	2461	2468	rVB	56545	87182	1.16%	0.223%

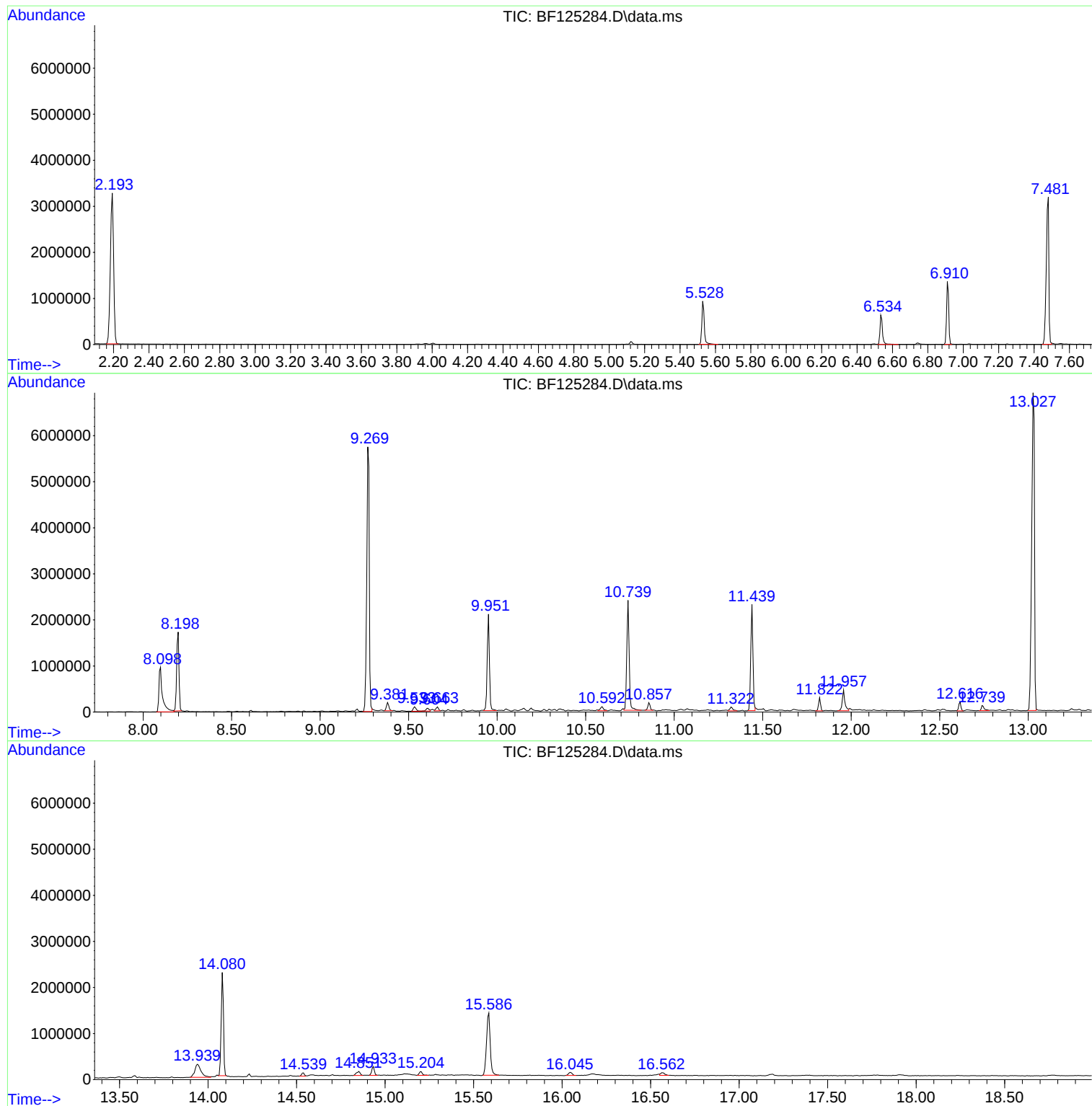
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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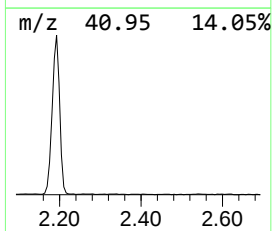
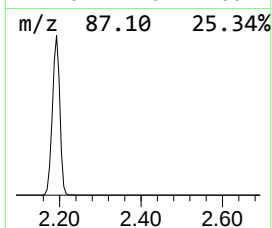
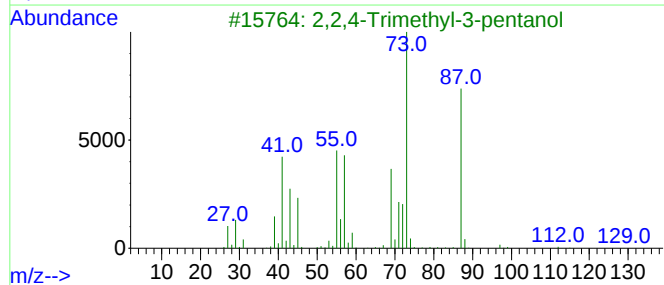
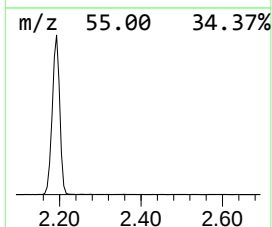
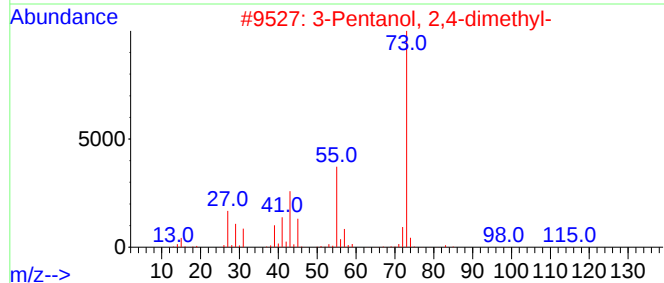
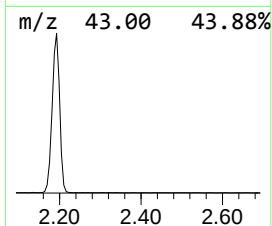
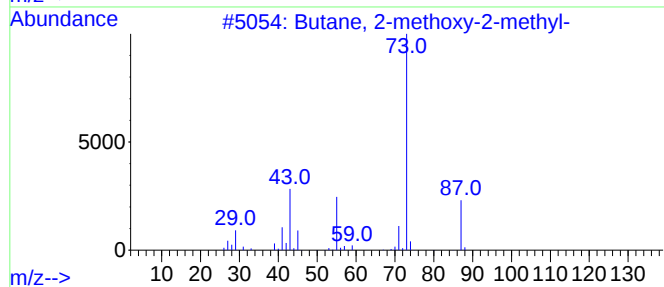
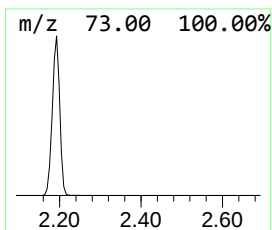
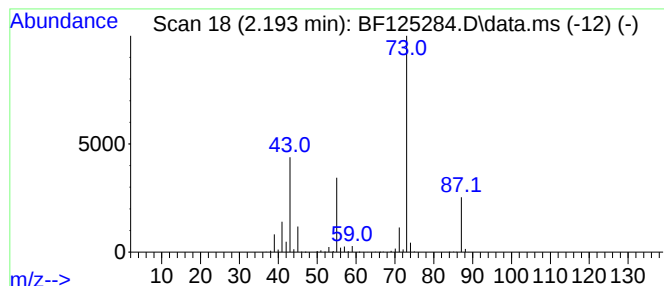
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	73.19 ng	4174030	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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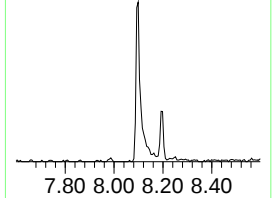
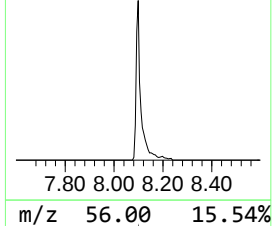
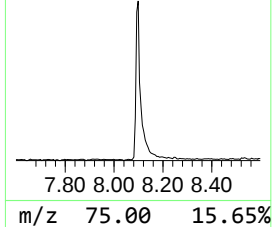
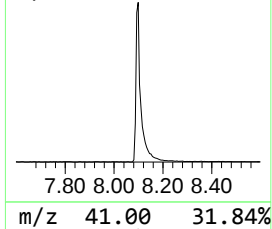
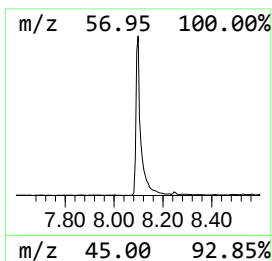
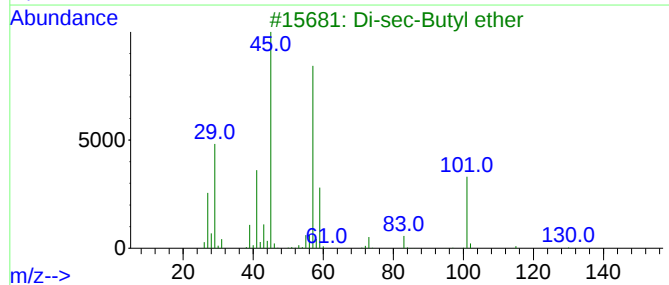
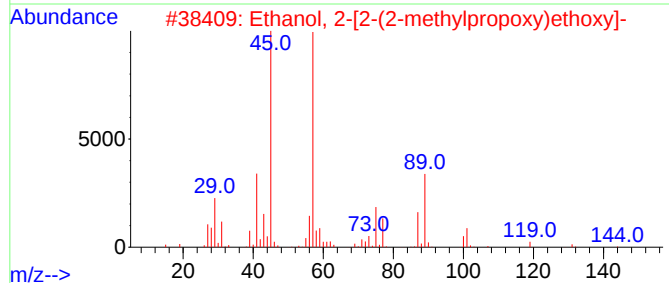
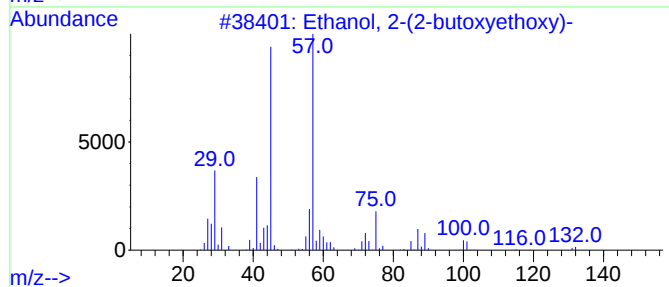
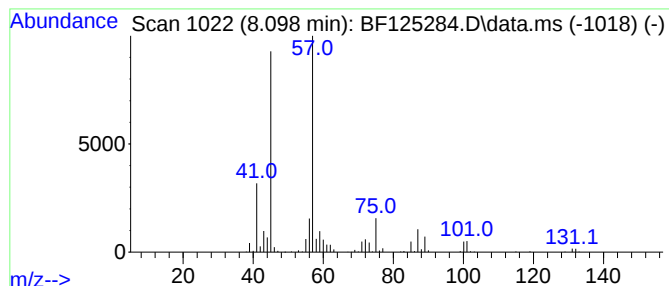
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	17.77 ng	1329830	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50



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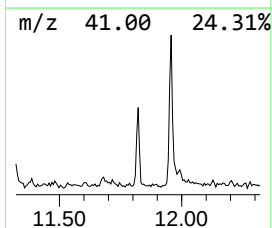
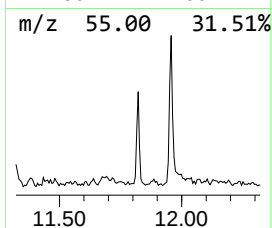
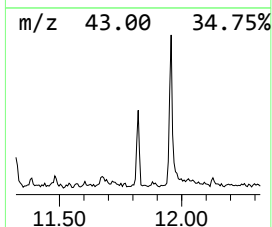
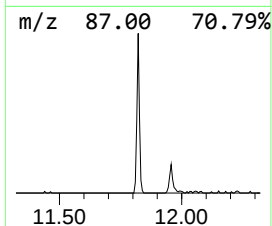
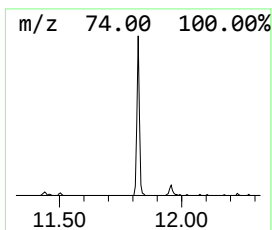
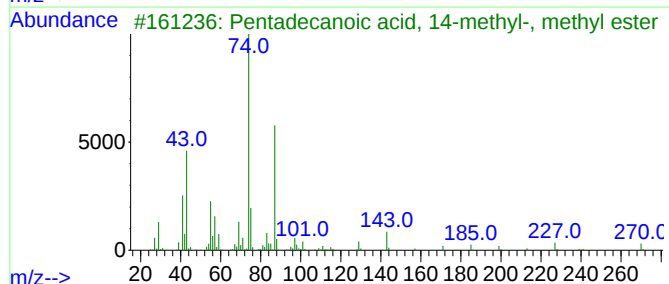
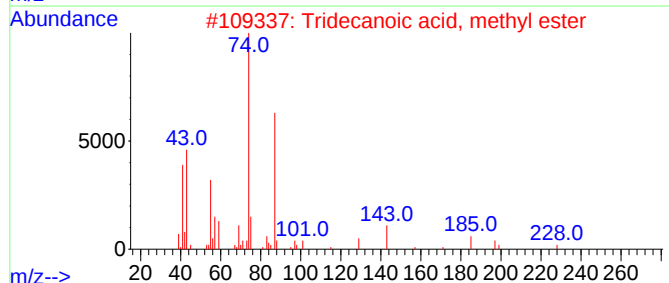
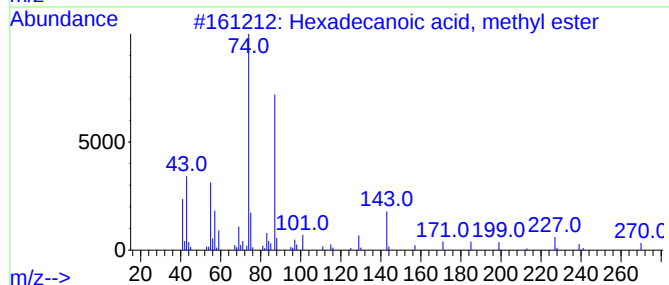
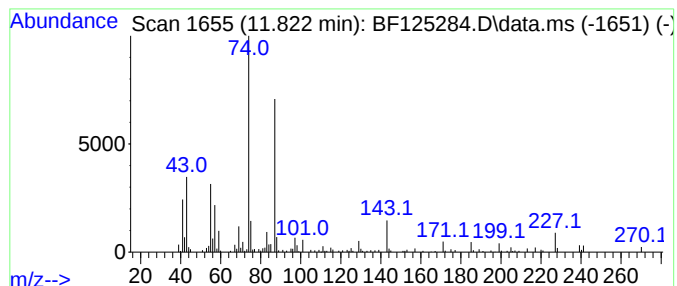
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	2.17 ng	212946	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80



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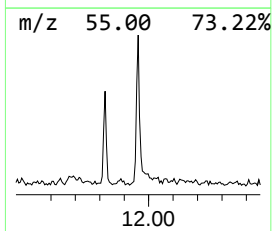
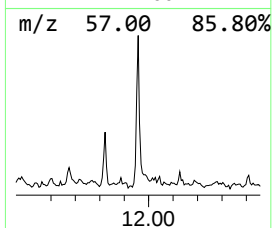
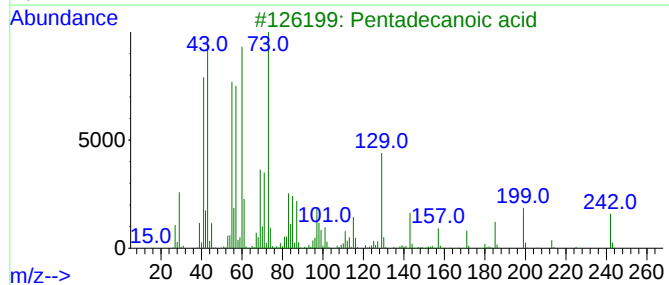
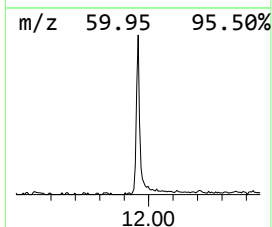
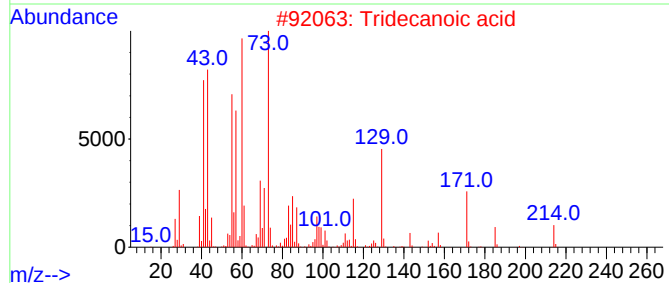
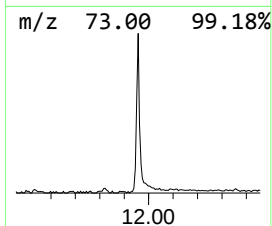
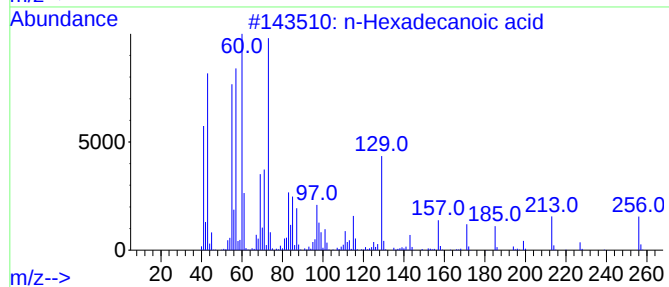
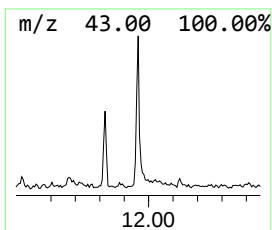
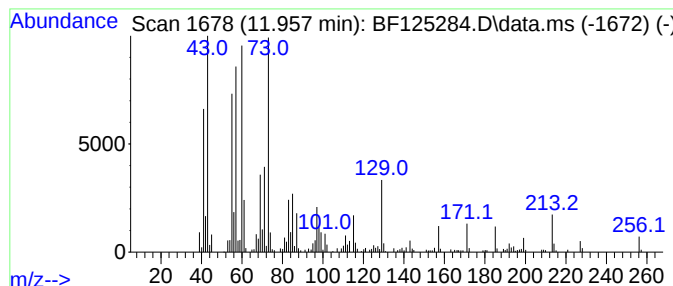
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	4.73 ng	465056	Phenanthrene-d10	11.439

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	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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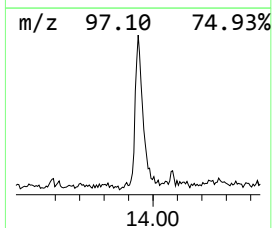
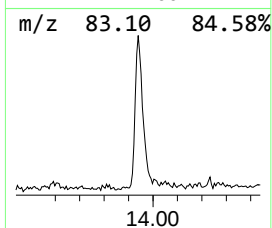
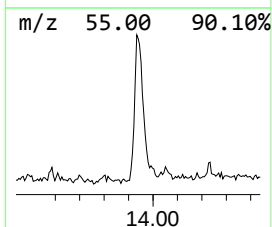
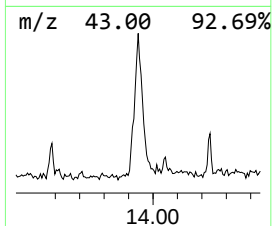
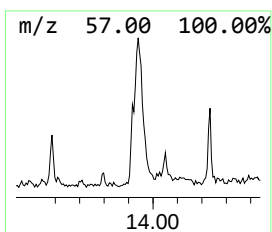
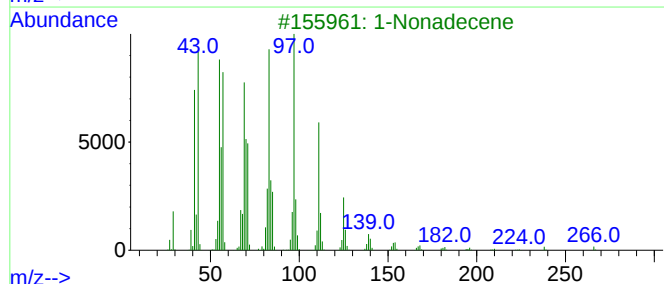
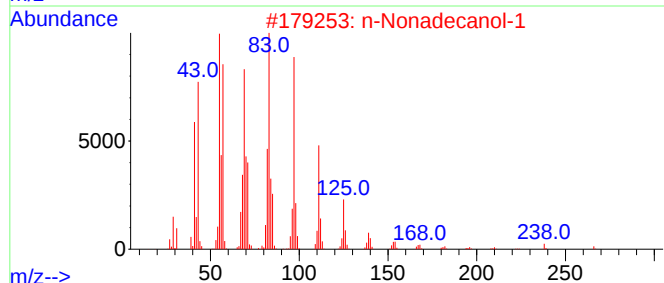
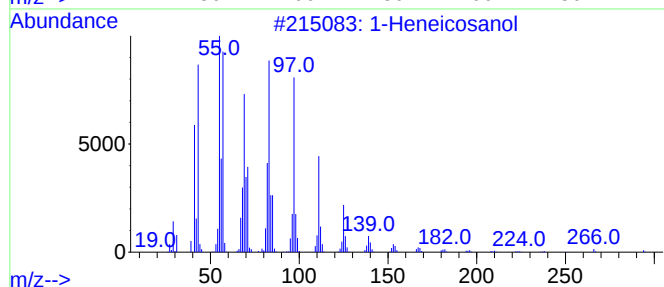
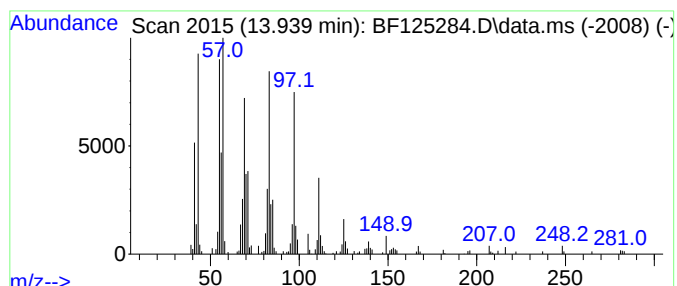
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Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.939	6.99 ng	697665	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	1-Octadecanol	270	C18H38O	000112-92-5	91
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	91



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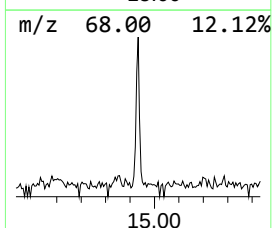
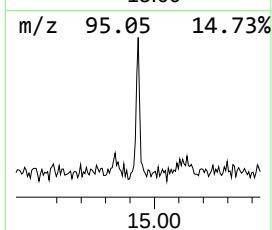
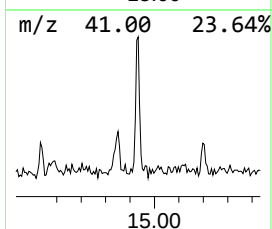
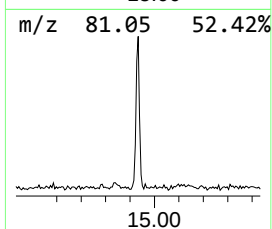
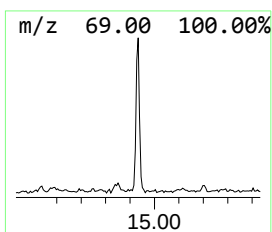
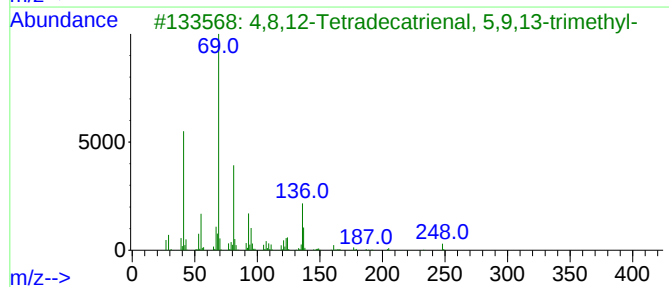
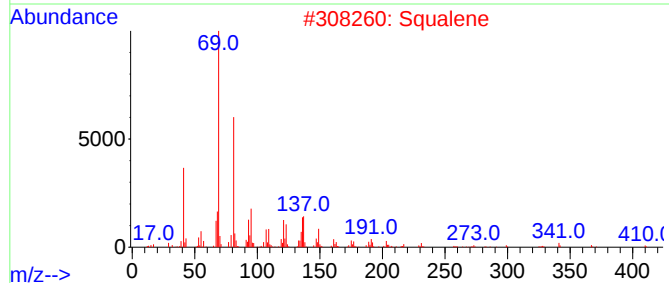
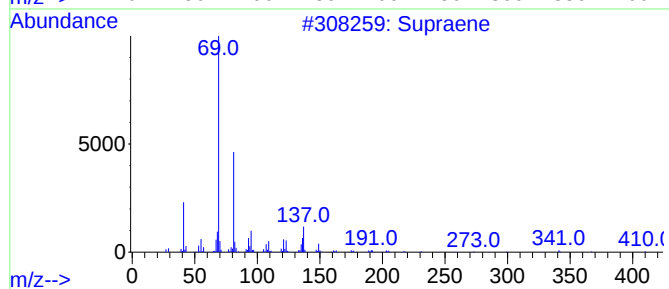
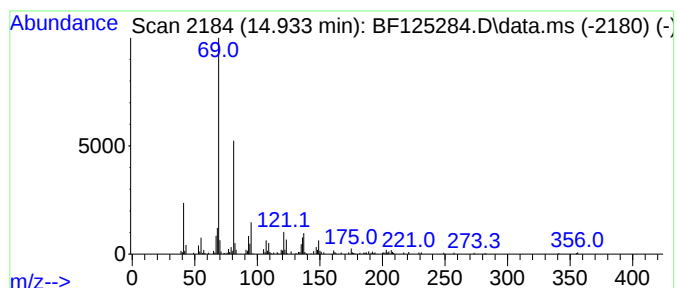
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	2.04 ng	200132	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene			410	C30H50	007683-64-9	91
2	Squalene			410	C30H50	000111-02-4	90
3	4,8,12-Tetradecatrienal, 5,9,13-...			248	C17H28O	066408-55-7	72
4	1,5,9-Decatriene, 2,3,5,8-tetram...			192	C14H24	230646-72-7	64
5	3,7,11-Trimethyl-2,6,10-dodecatr...			217	C15H23N	029789-67-1	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083121\
Data File : BF125284.D
Acq On : 31 Aug 2021 12:32
Operator : JU/CG
Sample : M3561-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EB-082621

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.193	73.2	ng	4174030	1	6.910	1140630	20.0
Ethanol, 2-(2-b...	8.098	17.8	ng	1329830	2	8.198	1496380	20.0
Hexadecanoic ac...	11.822	2.2	ng	212946	4	11.439	1967120	20.0
n-Hexadecanoic ...	11.957	4.7	ng	465056	4	11.439	1967120	20.0
1-Heneicosanol	13.939	7.0	ng	697665	5	14.080	1997590	20.0
Supraene	14.933	2.0	ng	200132	6	15.586	1958970	20.0