

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
 Data File : BF125194.D
 Acq On : 24 Aug 2021 20:04
 Operator : JU/CG
 Sample : M3430-05
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-5

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: BF125194.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	13	20	28	rVB	1318742	1677843	44.79%	5.810%
2	5.140	510	519	525	rVB	85921	106456	2.84%	0.369%
3	5.528	580	585	589	rBV	3209966	3285642	87.70%	11.378%
4	6.534	751	756	759	rBV	3244592	3286786	87.73%	11.382%
5	6.916	817	821	824	rBV	964167	847714	22.63%	2.935%
6	7.475	911	916	919	rBV	2488651	2147640	57.33%	7.437%
7	8.092	1018	1021	1035	rBV	745047	792939	21.17%	2.746%
8	8.198	1035	1039	1042	rVB	1241527	1084833	28.96%	3.757%
9	9.269	1217	1221	1224	rBV	4261421	3746298	100.00%	12.973%
10	9.951	1333	1337	1340	rBV	1535650	1223228	32.65%	4.236%
11	10.739	1466	1471	1474	rBV	2868587	2447081	65.32%	8.474%
12	11.439	1586	1590	1592	rBV	1355319	1207001	32.22%	4.180%
13	11.457	1592	1593	1597	rVB	113348	88862	2.37%	0.308%
14	11.957	1673	1678	1683	rBV2	273641	291030	7.77%	1.008%
15	12.651	1792	1796	1801	rBV	149649	140738	3.76%	0.487%
16	12.739	1808	1811	1816	rBV	74538	76739	2.05%	0.266%
17	12.839	1825	1828	1830	rBV	56421	42484	1.13%	0.147%
18	12.880	1830	1835	1839	rVB	123813	128702	3.44%	0.446%
19	13.021	1855	1859	1863	rBV	3779540	3392284	90.55%	11.747%
20	13.545	1945	1948	1952	rBV3	42842	46076	1.23%	0.160%
21	13.915	2008	2011	2013	rBV2	41405	45554	1.22%	0.158%
22	13.945	2013	2016	2017	rBV	79199	74891	2.00%	0.259%
23	14.074	2034	2038	2041	rBV	1016229	964475	25.74%	3.340%
24	14.104	2041	2043	2051	rVB	70088	67876	1.81%	0.235%
25	14.539	2114	2117	2122	rBV	41726	43207	1.15%	0.150%
26	14.610	2122	2129	2137	rBV8	56074	208737	5.57%	0.723%
27	15.127	2214	2217	2221	rBV2	55502	90720	2.42%	0.314%
28	15.204	2227	2230	2234	rVB	49232	50251	1.34%	0.174%
29	15.439	2267	2270	2275	rVB	35880	52761	1.41%	0.183%
30	15.504	2277	2281	2288	rVB	43893	56686	1.51%	0.196%
31	15.574	2288	2293	2302	rBV2	829224	1045913	27.92%	3.622%
32	16.051	2370	2374	2382	rVB2	42891	71954	1.92%	0.249%
33	17.533	2621	2626	2634	rVB5	20453	44738	1.19%	0.155%

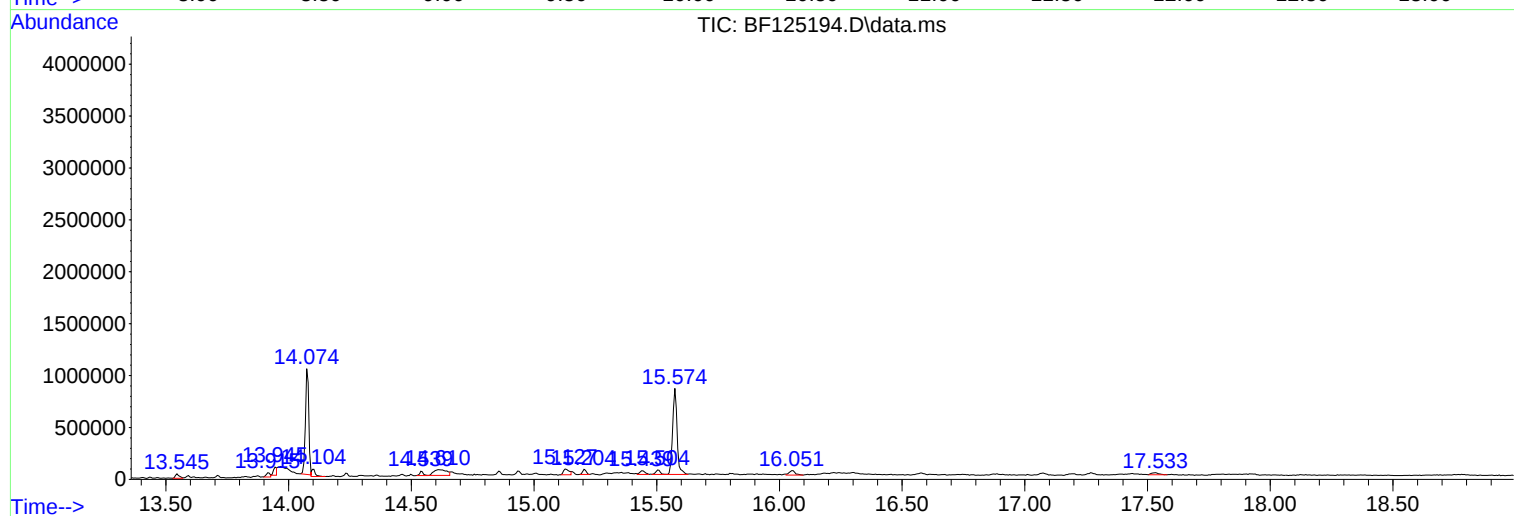
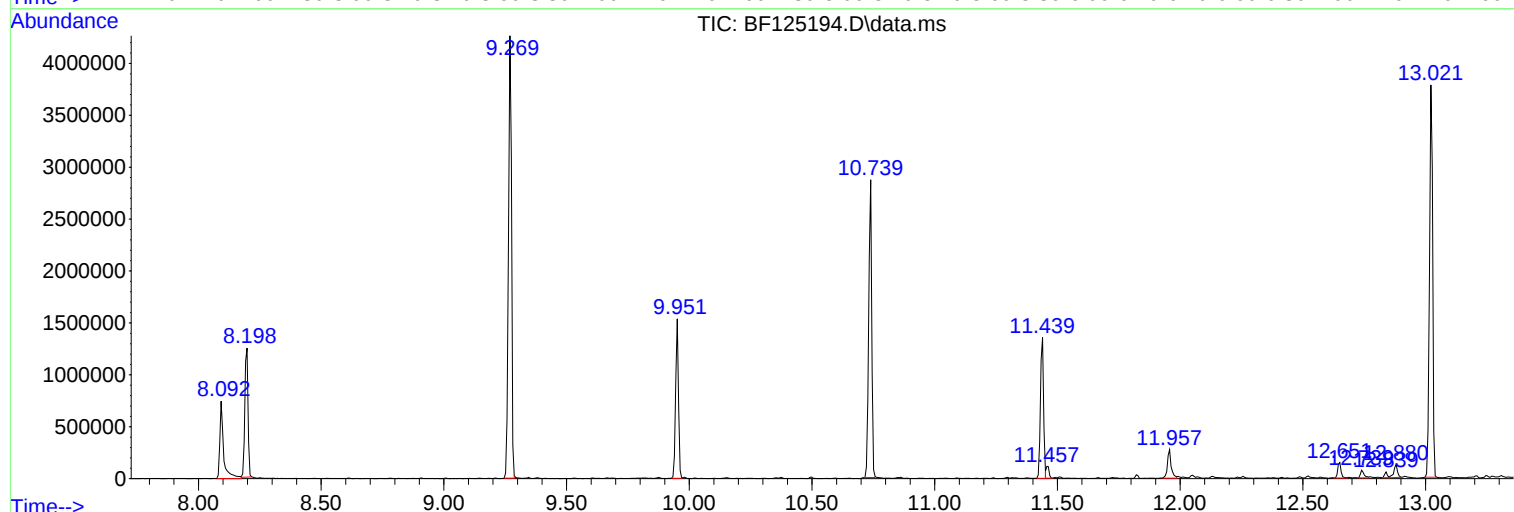
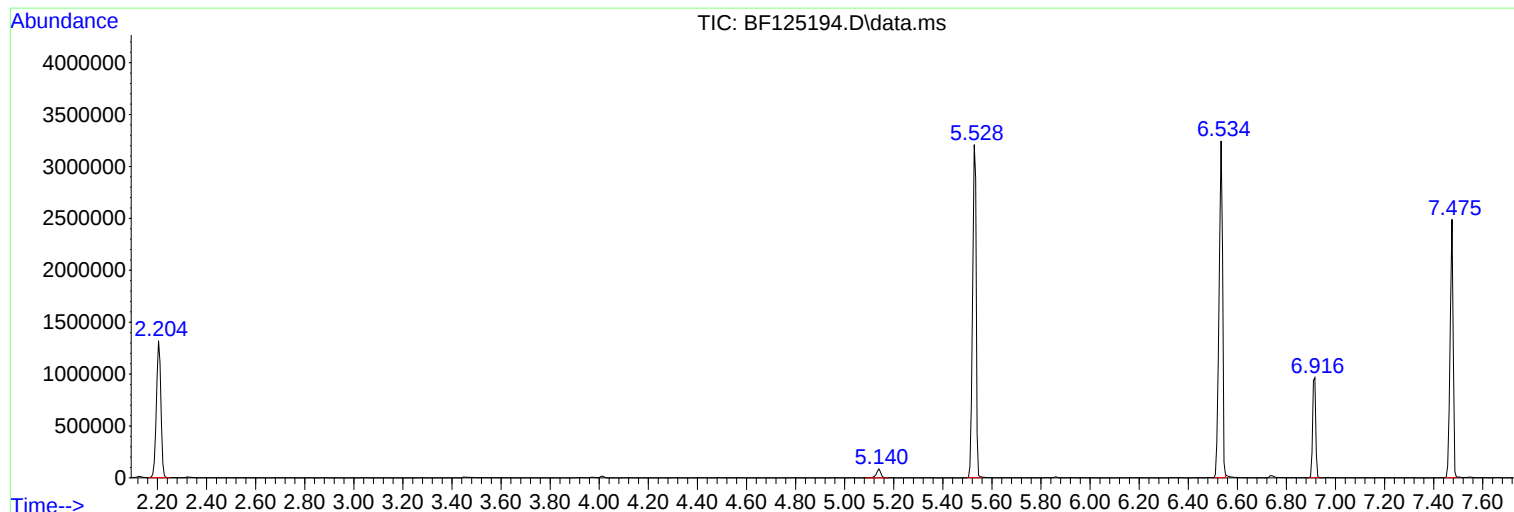
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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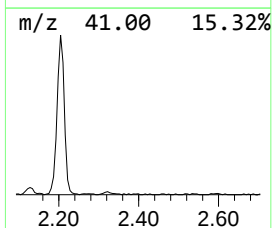
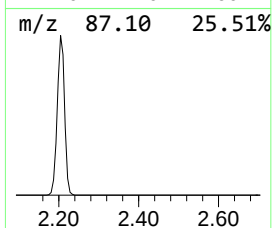
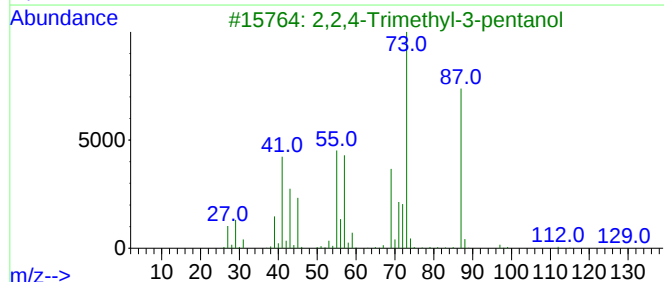
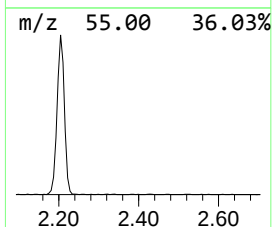
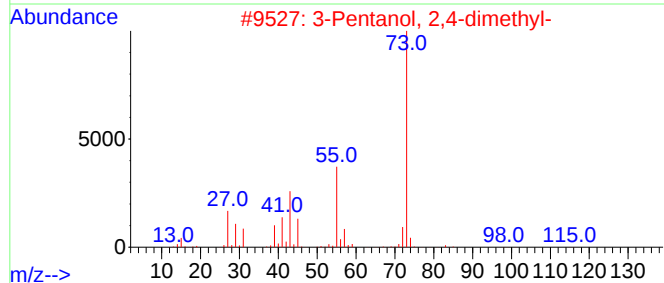
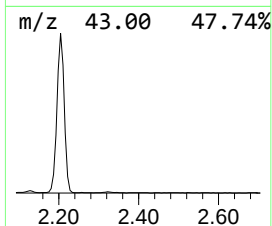
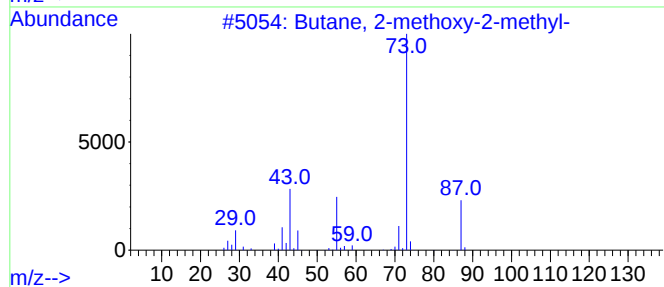
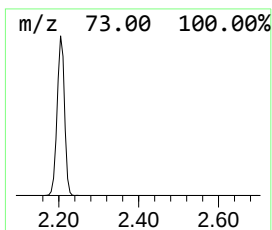
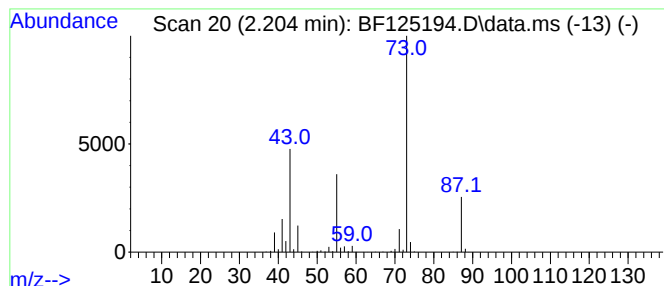
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	39.59 ng	1677840	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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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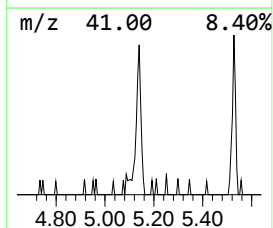
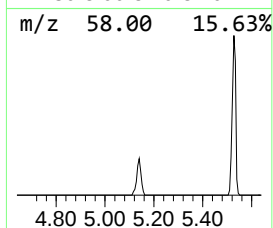
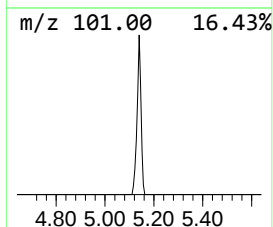
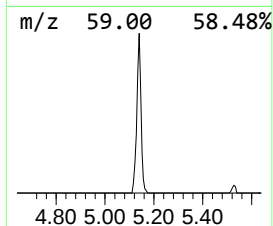
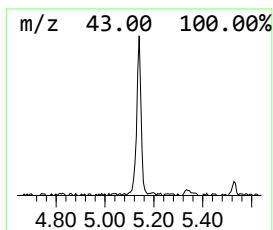
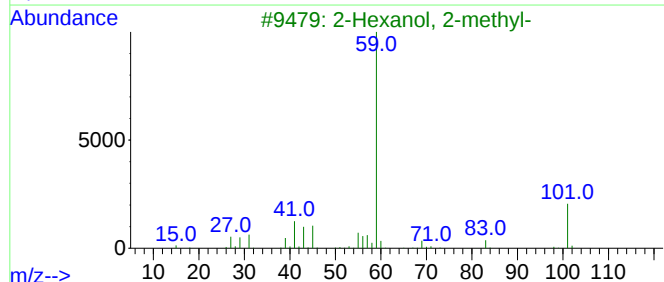
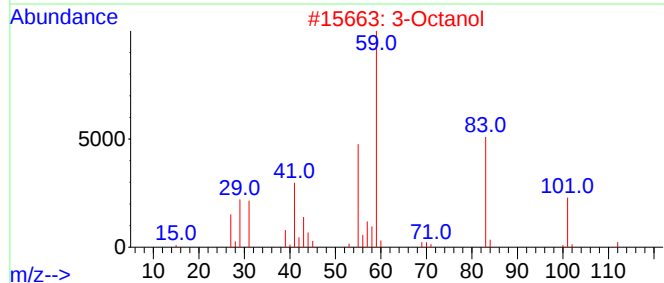
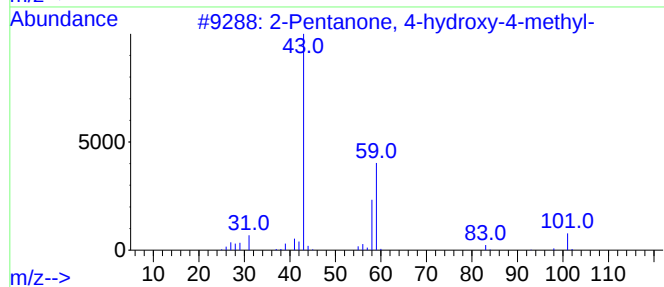
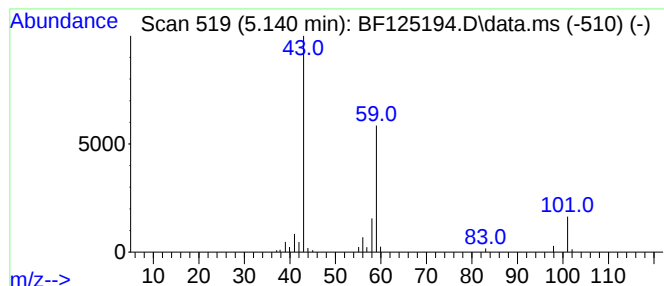
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	2.51 ng	106456	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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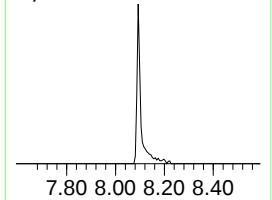
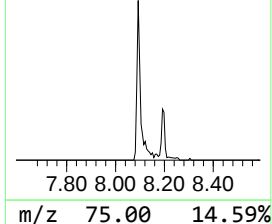
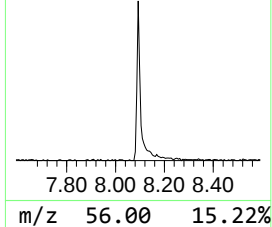
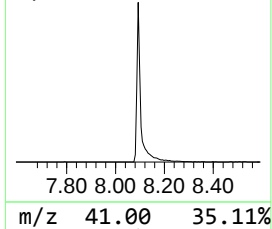
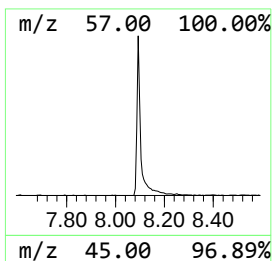
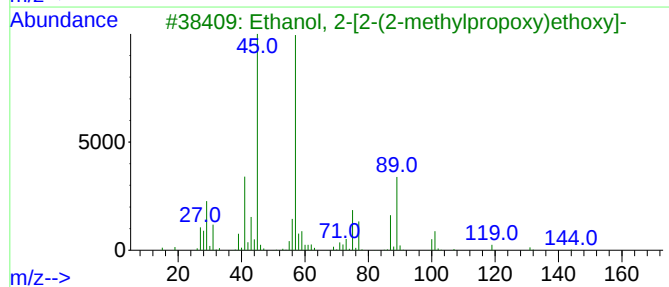
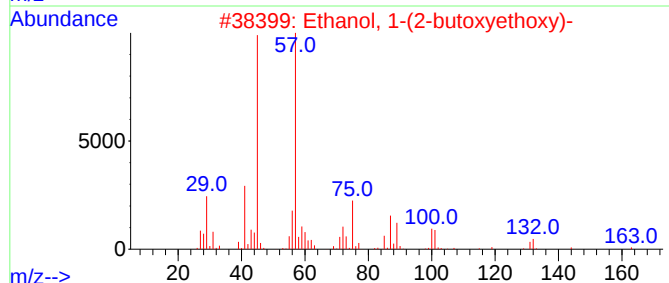
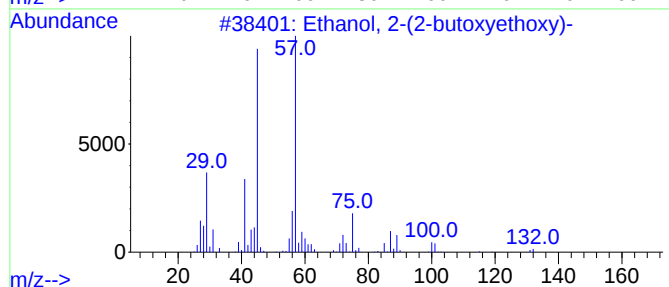
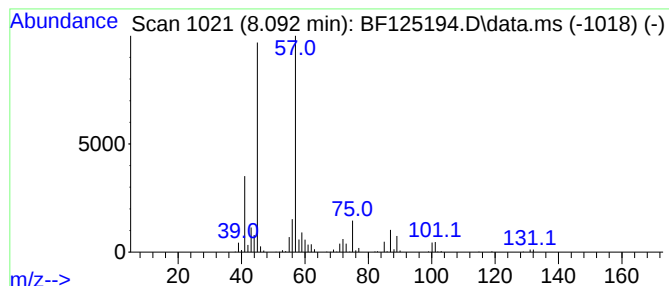
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	14.62 ng	792939	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, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50
5			2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	50



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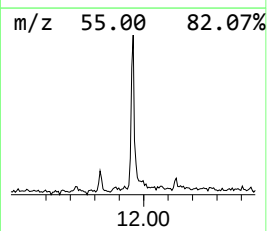
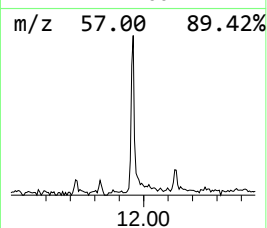
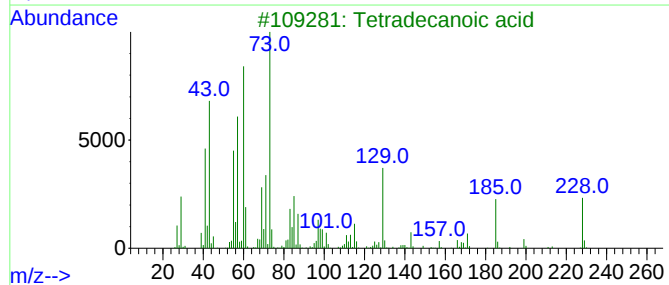
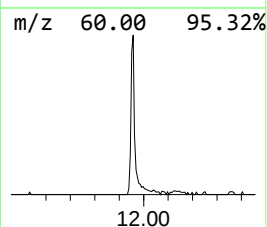
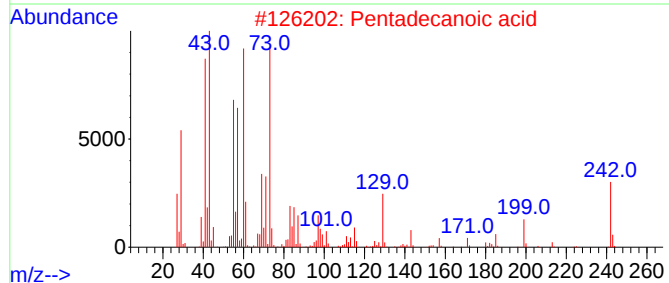
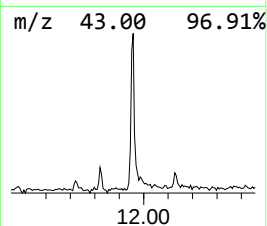
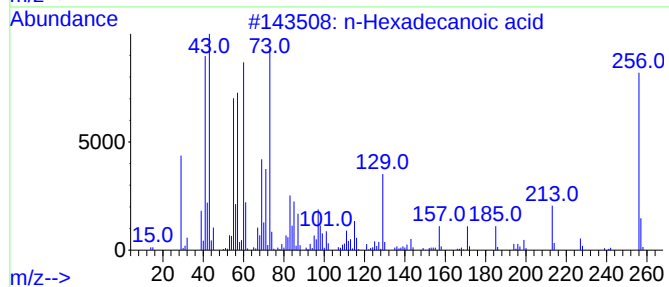
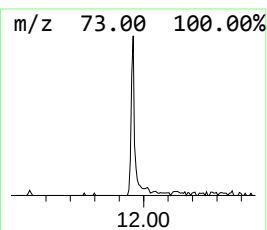
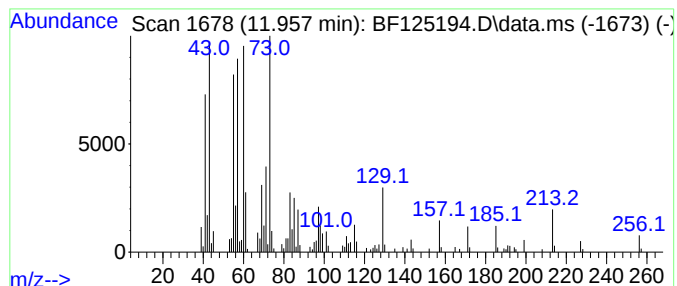
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	4.82 ng	291030	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



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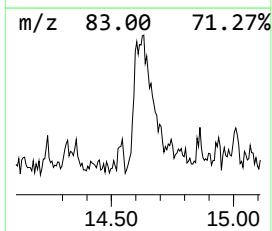
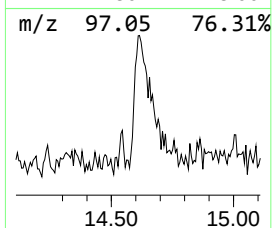
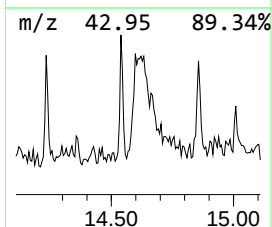
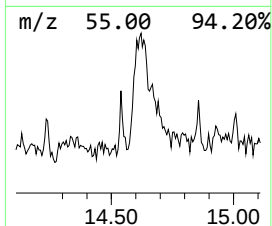
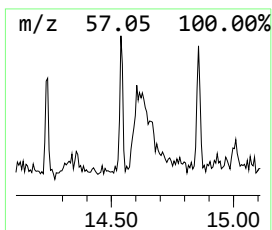
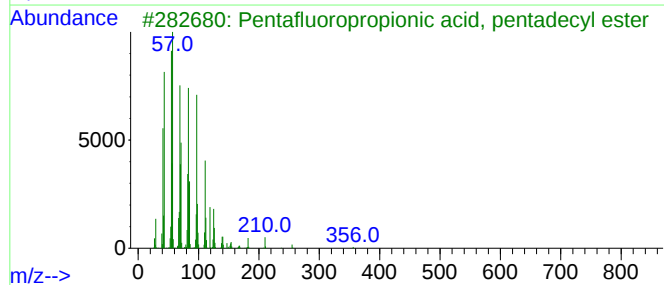
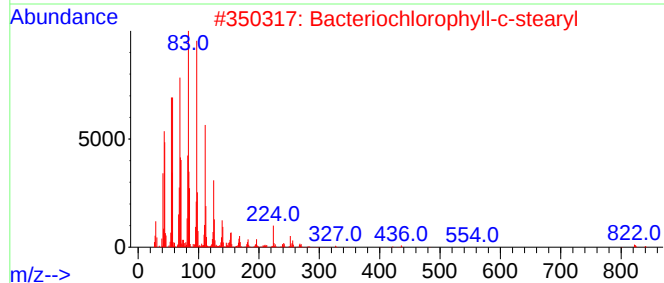
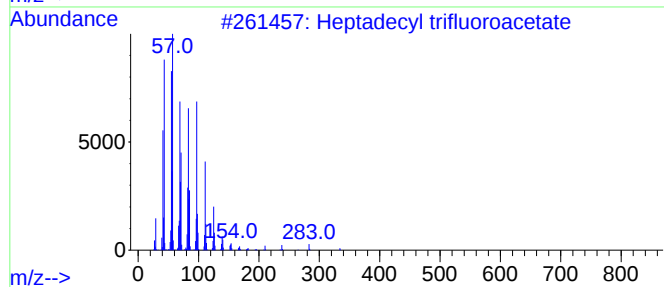
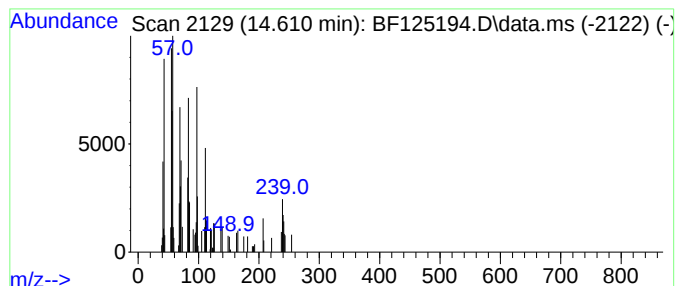
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Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.610	4.33 ng	208737	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	76
2			Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1010164-49-7	68
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	64
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	64
5			3-Chloropropionic acid, octadecy...	360	C21H41ClO2	088168-99-4	64



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PE-5

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...	2.204	39.6	ng	1677840	1	6.916	847714	20.0
2-Pentanone, 4-...	5.140	2.5	ng	106456	1	6.916	847714	20.0
Ethanol, 2-(2-b...	8.092	14.6	ng	792939	2	8.198	1084830	20.0
n-Hexadecanoic ...	11.957	4.8	ng	291030	4	11.439	1207000	20.0
Heptadecyl trif...	14.610	4.3	ng	208737	5	14.074	964475	20.0