

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
 Data File : BF125929.D
 Acq On : 26 Oct 2021 12:09
 Operator : JU/CG
 Sample : M4325-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RED-BOX-1-225057

Integration Parameters: rteint.p

Integrator: RTE

Smothing : 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-BF102521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125929.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	15	21	rVB	2941024	3918573	75.13%	9.391%
2	3.357	214	216	227	rBV	29220	60414	1.16%	0.145%
3	5.104	510	513	521	rVB	48135	64303	1.23%	0.154%
4	5.487	572	578	581	rBV	4807764	5160205	98.93%	12.366%
5	6.493	742	749	752	rBV	4505173	5210983	99.91%	12.488%
6	6.863	809	812	815	rBV	1090785	946347	18.14%	2.268%
7	7.428	902	908	911	rBV	3570045	3446228	66.07%	8.259%
8	8.051	1010	1014	1018	rBV	1551388	1360555	26.08%	3.260%
9	8.145	1026	1030	1034	rBV	1395214	1276761	24.48%	3.060%
10	9.228	1208	1214	1217	rBV	5550336	4981142	95.50%	11.937%
11	9.904	1325	1329	1332	rVB	1637124	1408266	27.00%	3.375%
12	10.692	1455	1463	1466	rBV	3906951	3743165	71.76%	8.970%
13	11.386	1577	1581	1584	rBV	1873754	1516460	29.07%	3.634%
14	11.457	1587	1593	1596	rBV2	67001	66279	1.27%	0.159%
15	11.786	1646	1649	1653	rVB	71064	55469	1.06%	0.133%
16	11.916	1666	1671	1675	rBV	363254	338802	6.50%	0.812%
17	12.704	1800	1805	1811	rBV	121110	136430	2.62%	0.327%
18	12.980	1847	1852	1855	rBV	5449746	5215866	100.00%	12.500%
19	13.874	1999	2004	2011	rBV2	364799	414463	7.95%	0.993%
20	14.021	2025	2029	2033	rBV	1290049	1260697	24.17%	3.021%
21	14.510	2109	2112	2117	rBV	59678	59167	1.13%	0.142%
22	14.898	2175	2178	2183	rBV	108701	116725	2.24%	0.280%
23	15.492	2274	2279	2286	rVV	742402	904301	17.34%	2.167%
24	15.557	2286	2290	2296	rVB2	43111	66888	1.28%	0.160%

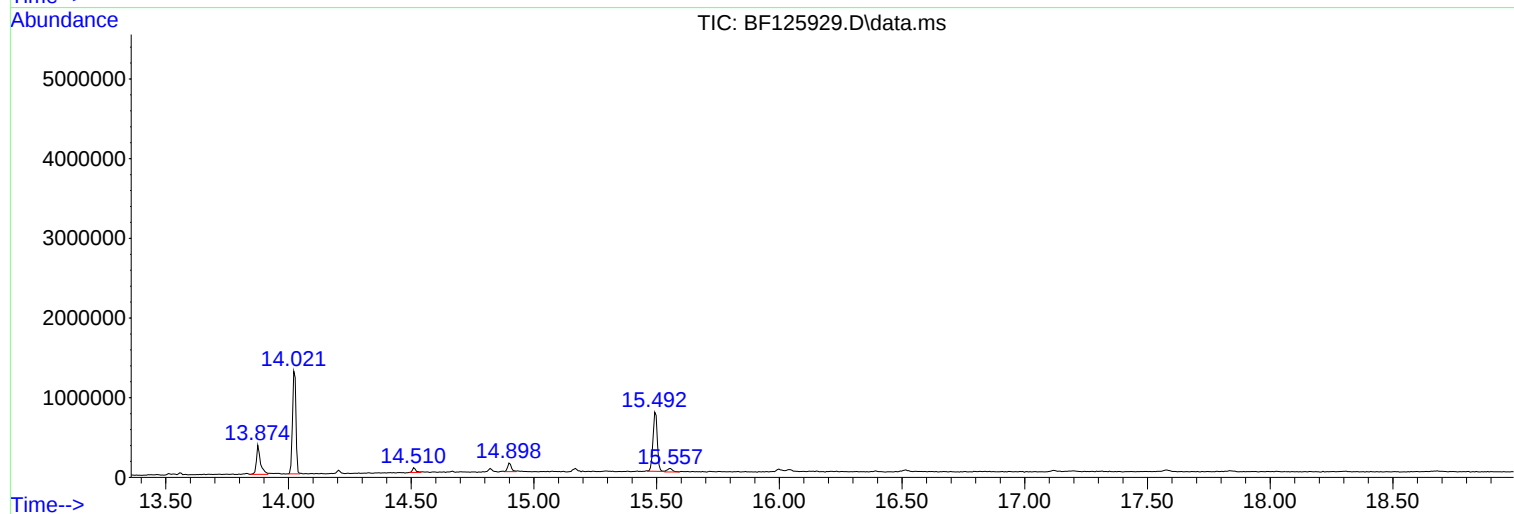
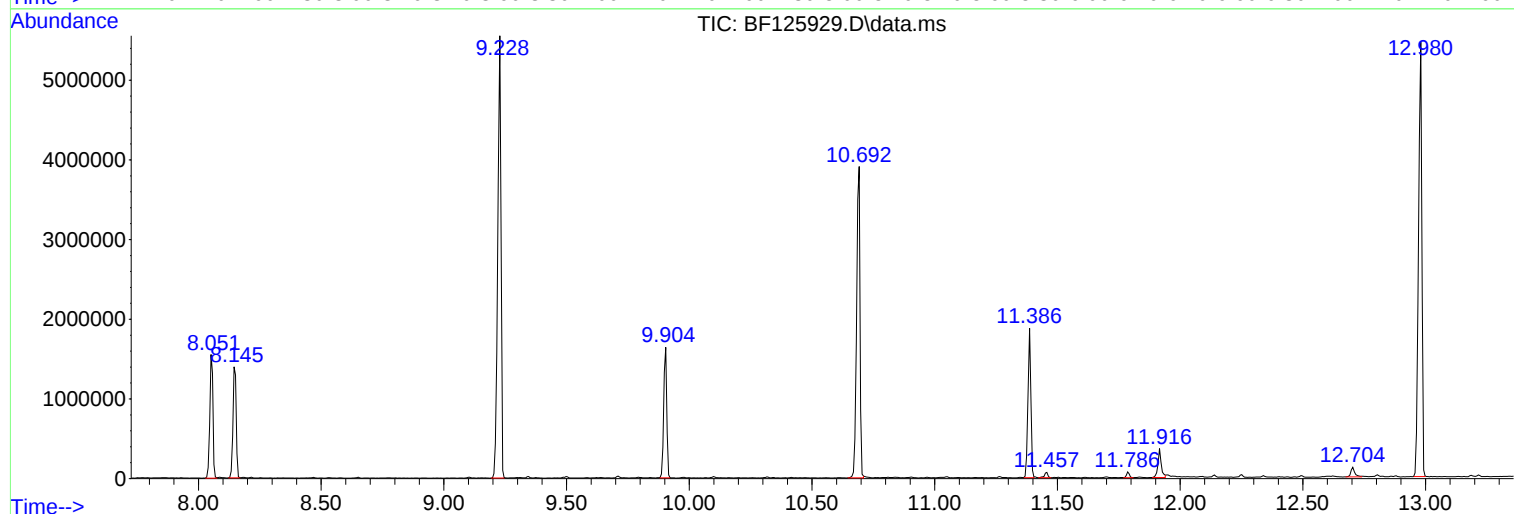
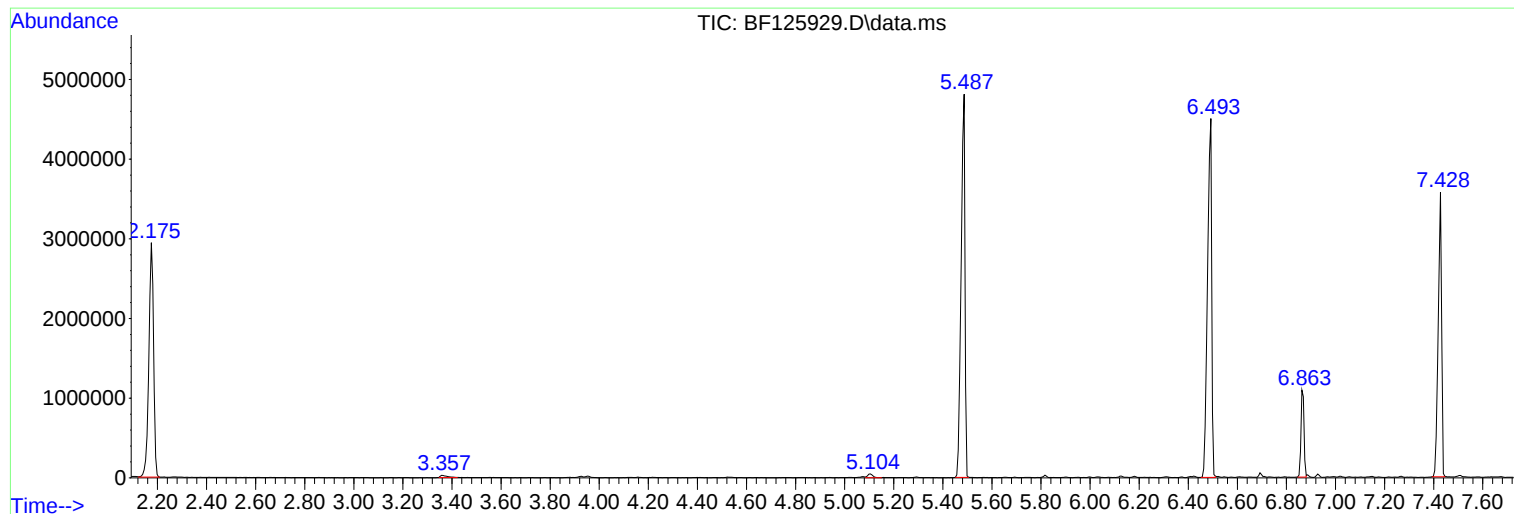
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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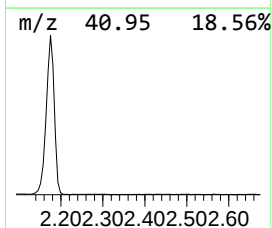
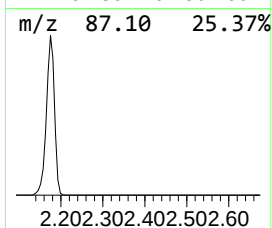
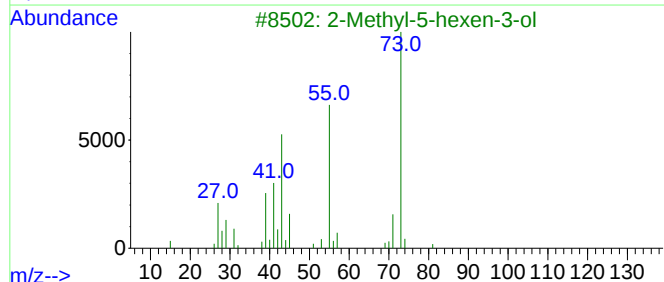
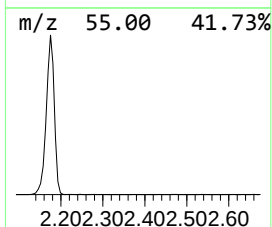
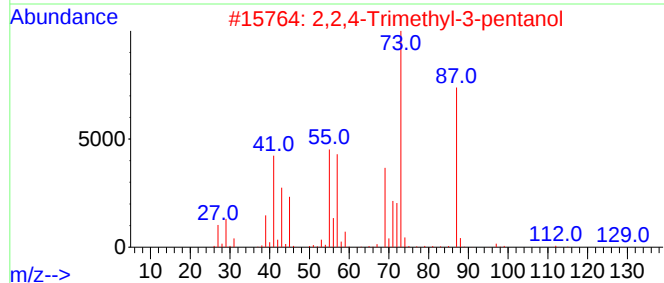
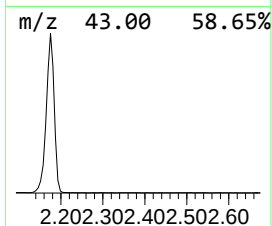
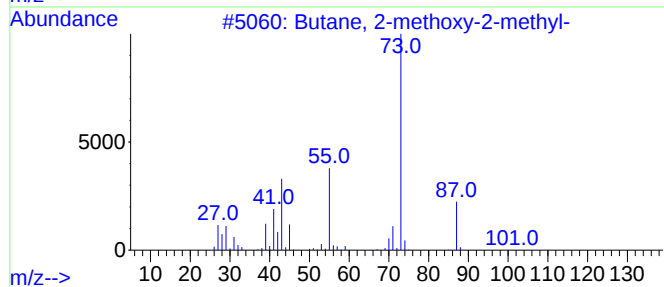
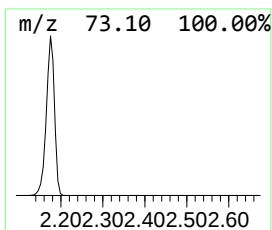
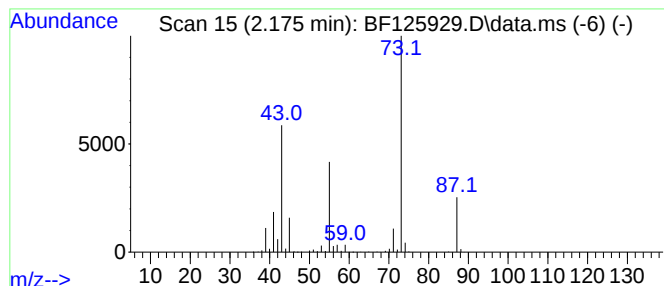
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	82.81 ng	3918570	1,4-Dichlorobenzene-d4	6.869

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			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	25



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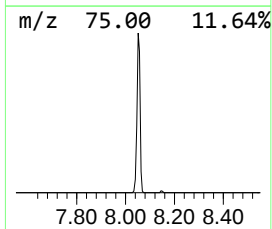
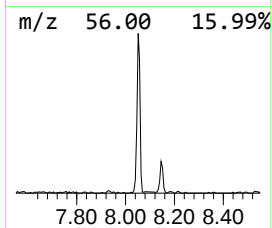
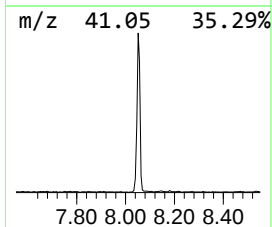
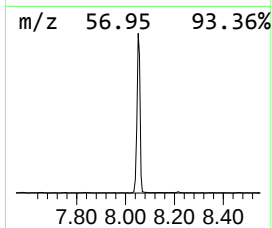
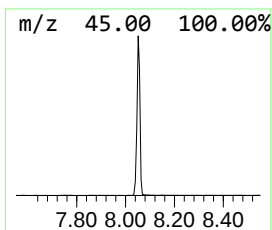
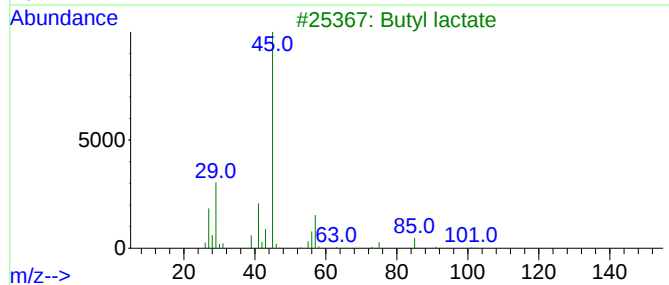
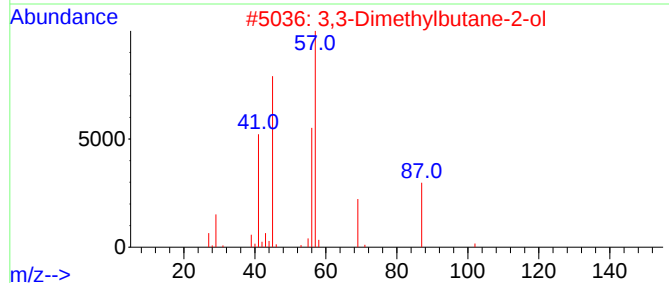
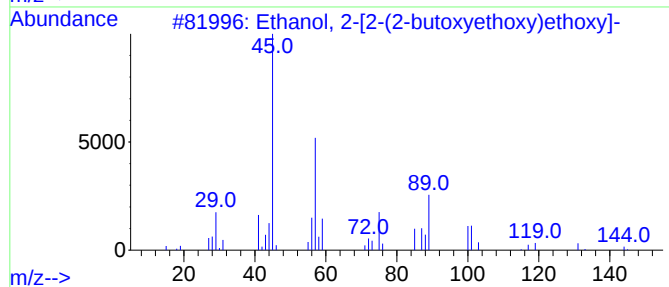
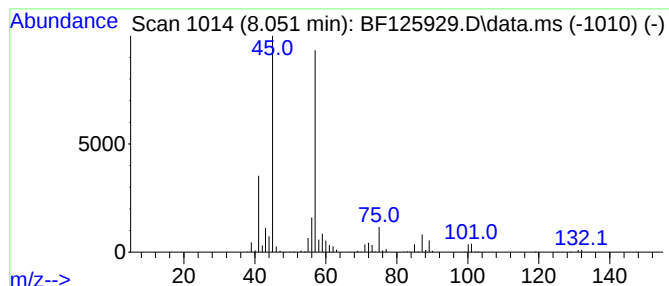
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-[2-(2-butoxyetho... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	21.31 ng	1360560	Naphthalene-d8	8.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
2			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
3			Butyl lactate	146	C7H14O3	000138-22-7	50
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	47



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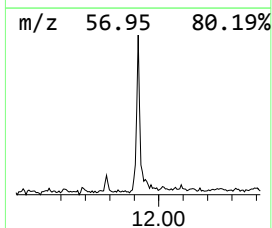
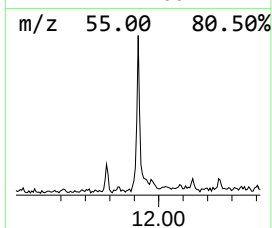
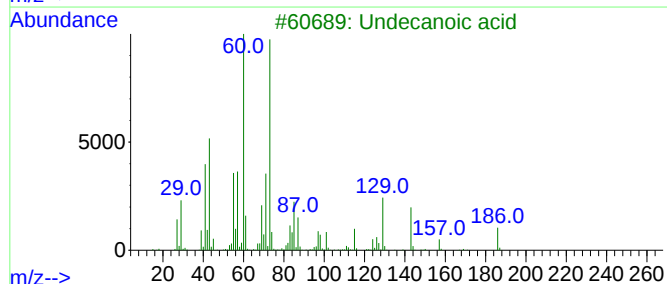
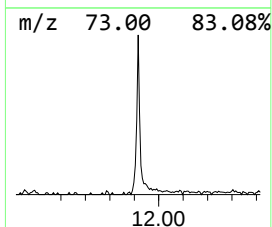
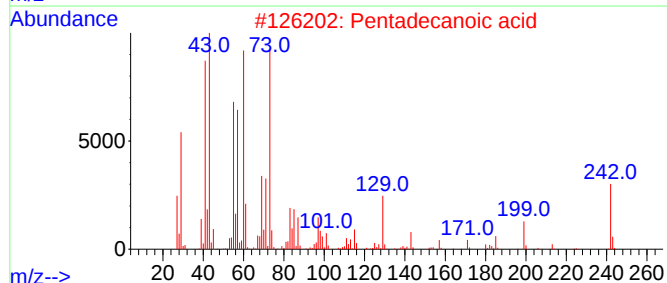
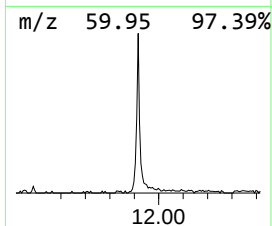
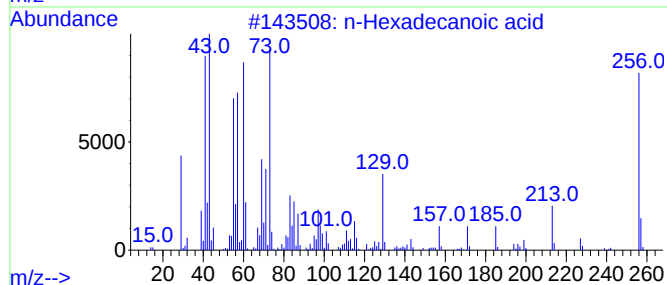
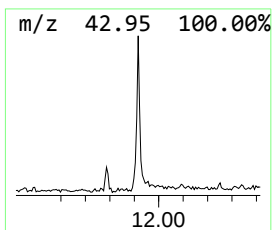
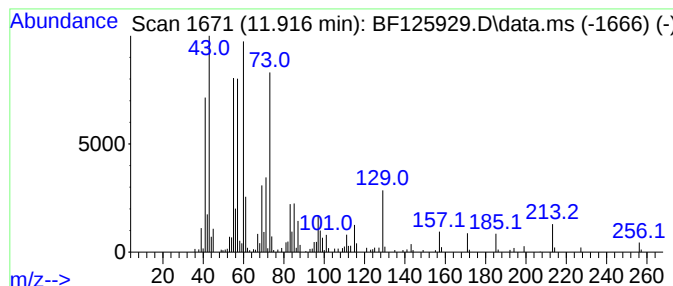
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	4.47 ng	338802	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Undecanoic acid	186	C11H22O2	000112-37-8	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



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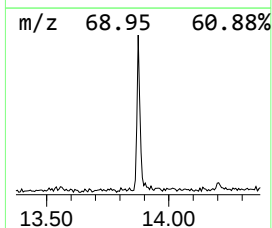
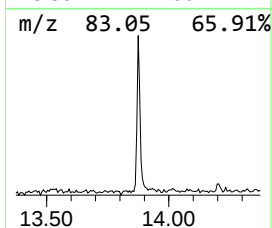
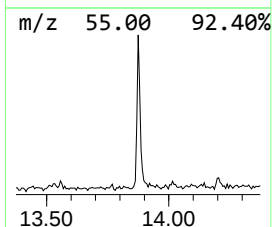
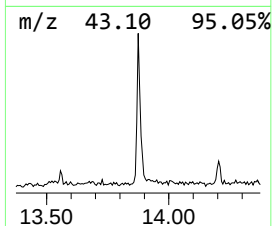
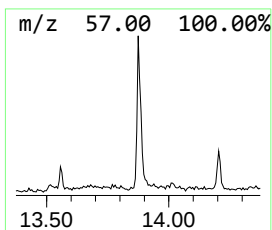
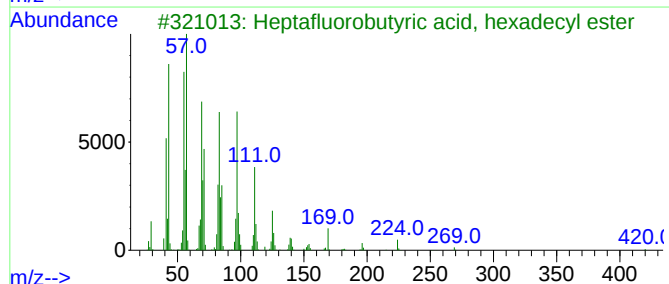
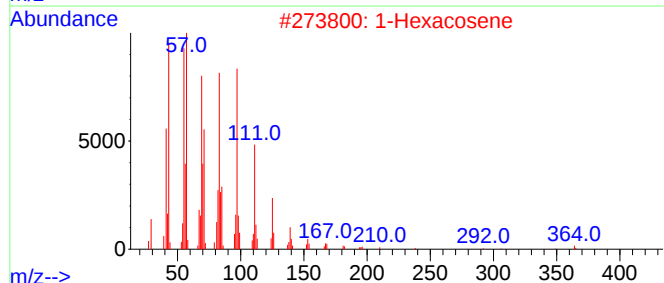
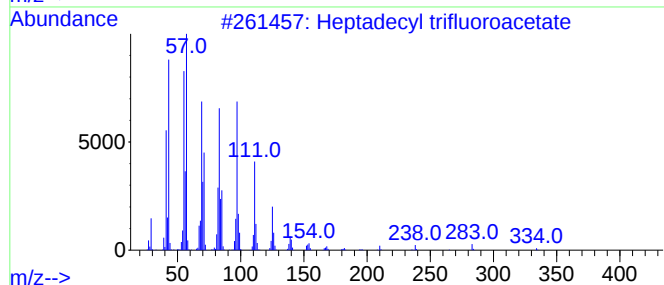
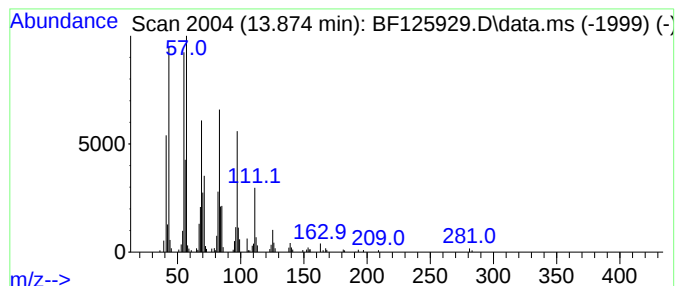
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Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.58 ng	414463	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2			1-Hexacosene	364	C26H52	018835-33-1	91
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
4			1-Octadecanol	270	C18H38O	000112-92-5	91
5			Octacosanol	410	C28H58O	000557-61-9	91



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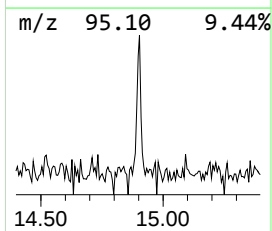
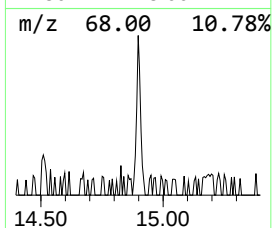
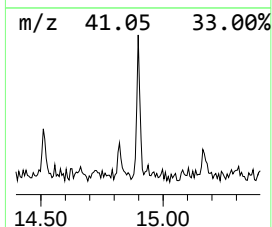
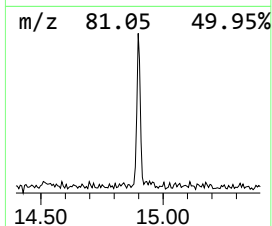
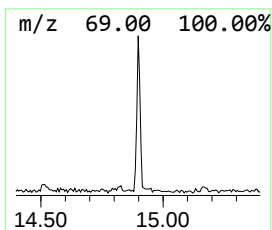
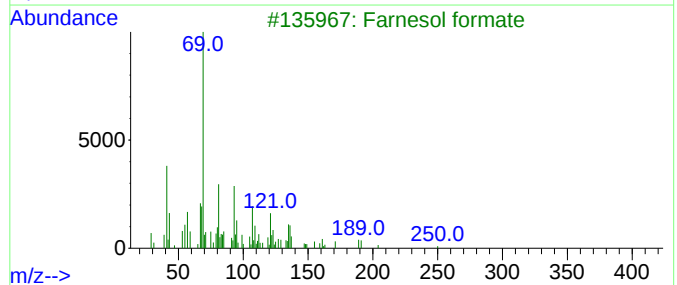
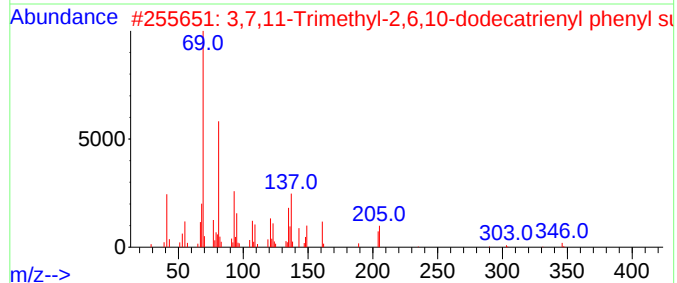
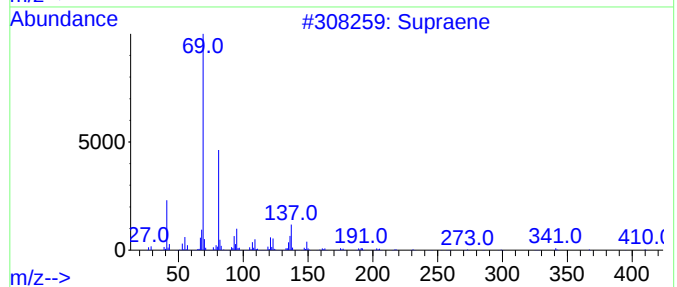
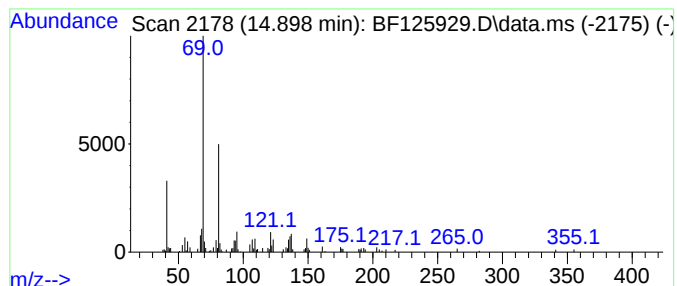
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.58 ng	116725	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			3,7,11-Trimethyl-2,6,10-dodecatr...	346	C21H30O2S	1000432-39-0	72
3			Farnesol formate	250	C16H26O2	917105-98-7	64
4			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	64
5			trans-Farnesol	222	C15H26O	000106-28-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	82.8	ng	3918570	1	6.869	946347	20.0
Ethanol, 2-[2-(...	8.051	21.3	ng	1360560	2	8.145	1276760	20.0
n-Hexadecanoic ...	11.916	4.5	ng	338802	4	11.386	1516460	20.0
Heptadecyl trif...	13.874	6.6	ng	414463	5	14.027	1260700	20.0
Supraene	14.898	2.6	ng	116725	6	15.492	904301	20.0