

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
 Data File : BF125944.D
 Acq On : 26 Oct 2021 20:39
 Operator : JU/CG
 Sample : M4348-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 354

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-BF102521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125944.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	20	rVB	2871665	3813769	95.60%	12.579%
2	5.093	507	511	518	rVB	41706	56210	1.41%	0.185%
3	5.481	572	577	580	rBV	4276406	3973671	99.61%	13.107%
4	6.487	742	748	751	rBV	4075901	3989104	100.00%	13.158%
5	6.863	807	812	816	rBV	1354079	1125895	28.22%	3.714%
6	7.422	902	907	910	rBV	2823129	2596057	65.08%	8.563%
7	8.051	1010	1014	1017	rBV	817574	587318	14.72%	1.937%
8	8.145	1026	1030	1034	rBV	1613876	1434065	35.95%	4.730%
9	9.222	1209	1213	1216	rBV	3333589	2847995	71.39%	9.394%
10	9.904	1325	1329	1332	rBV	1714706	1535350	38.49%	5.064%
11	10.310	1395	1398	1401	rBV	35819	41169	1.03%	0.136%
12	10.686	1458	1462	1465	rBV	2888574	2479567	62.16%	8.179%
13	11.386	1577	1581	1584	rBV	1868889	1536211	38.51%	5.067%
14	11.457	1587	1593	1595	rVB4	52249	55367	1.39%	0.183%
15	11.916	1665	1671	1682	rBV	209995	220499	5.53%	0.727%
16	12.698	1801	1804	1810	rBV2	63179	65321	1.64%	0.215%
17	12.969	1846	1850	1854	rBV	1963779	1837514	46.06%	6.061%
18	13.874	2000	2004	2010	rBV	171022	162466	4.07%	0.536%
19	14.021	2025	2029	2032	rBV	1054015	893626	22.40%	2.948%
20	14.898	2174	2178	2183	rBV	118605	117466	2.94%	0.387%
21	15.492	2274	2279	2285	rVB	834831	949268	23.80%	3.131%

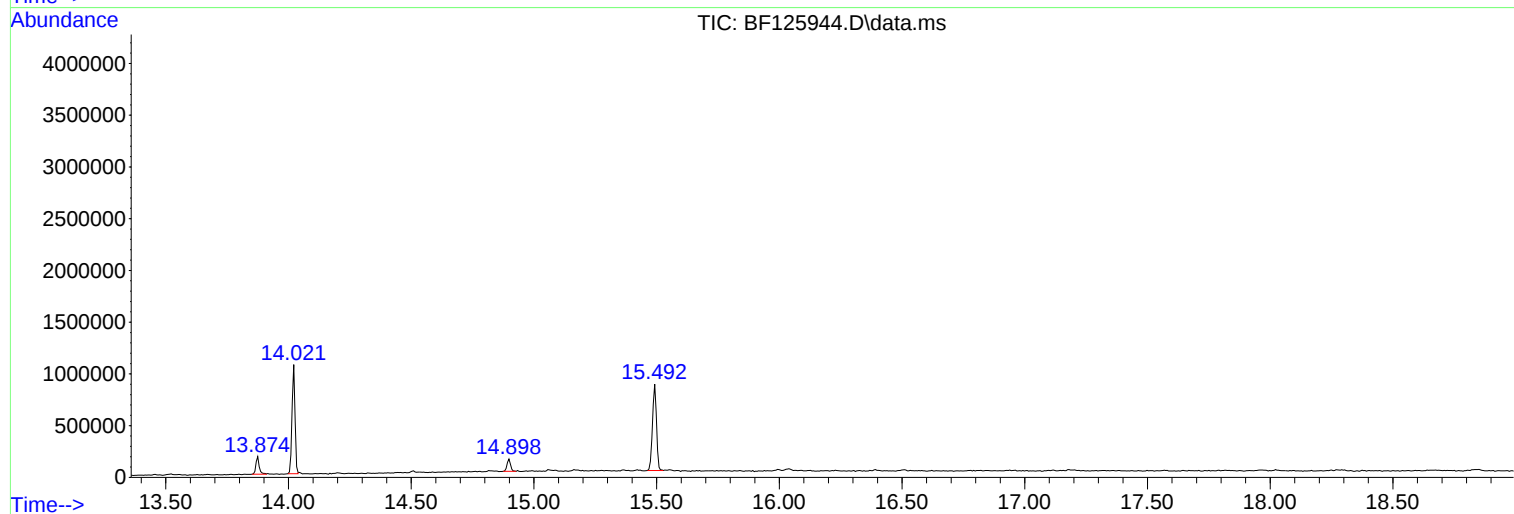
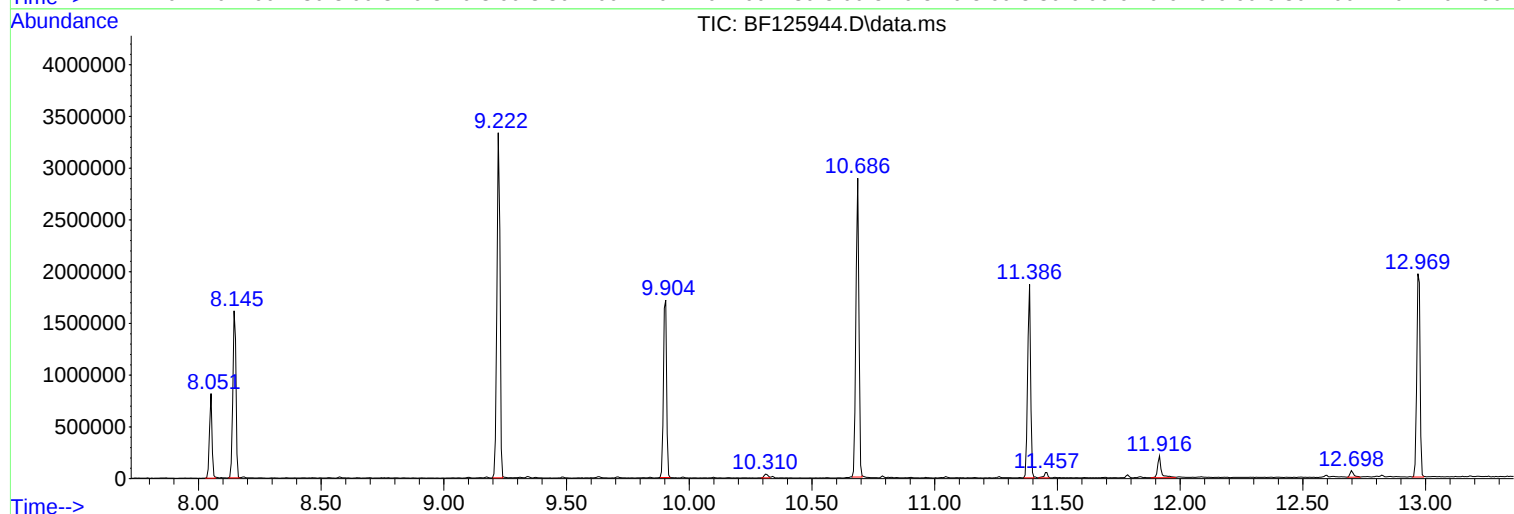
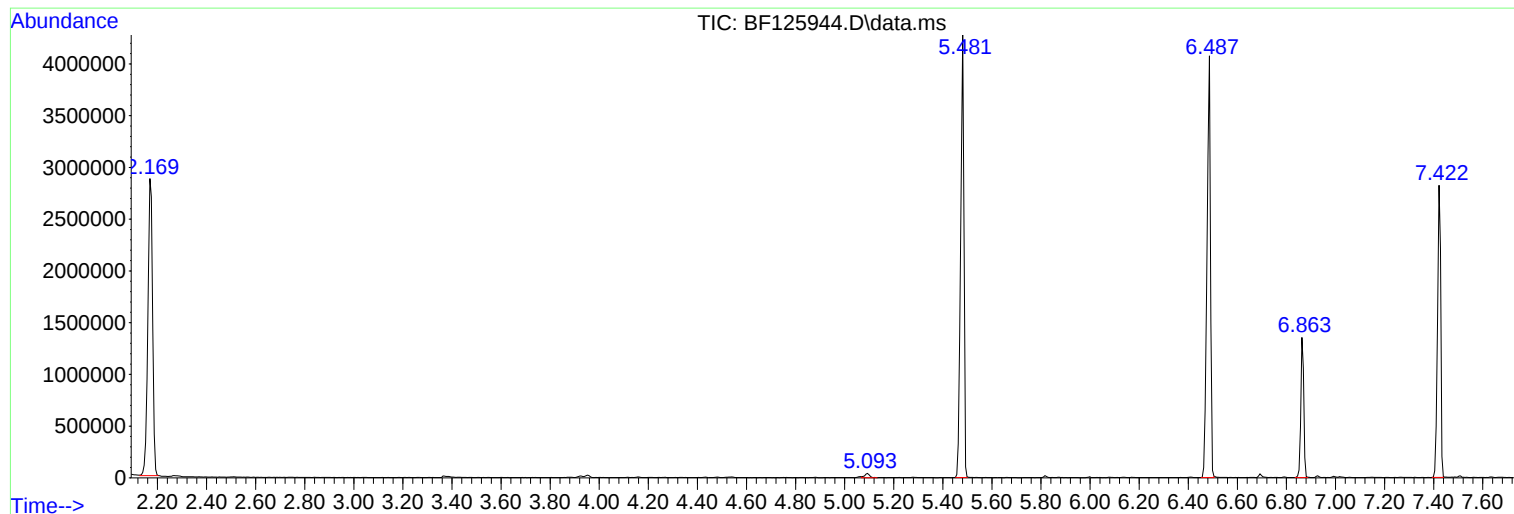
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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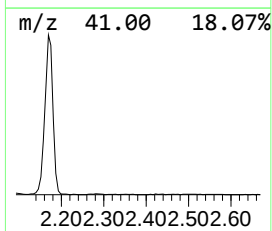
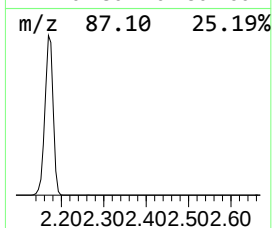
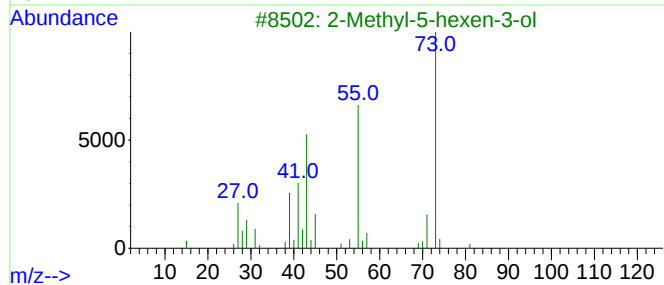
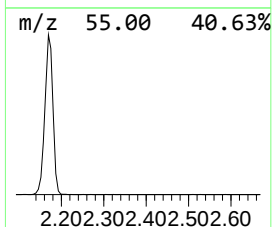
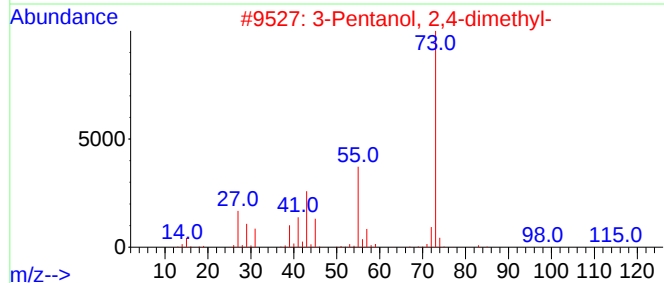
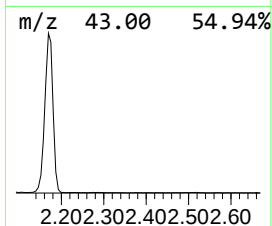
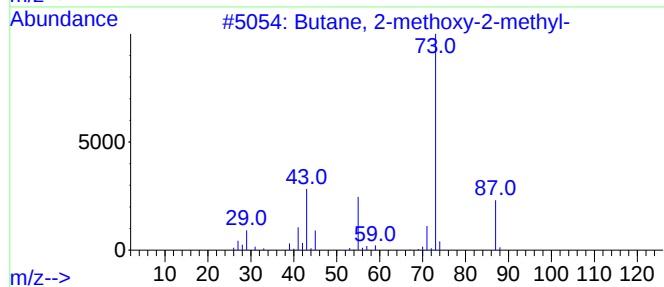
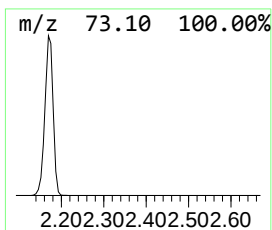
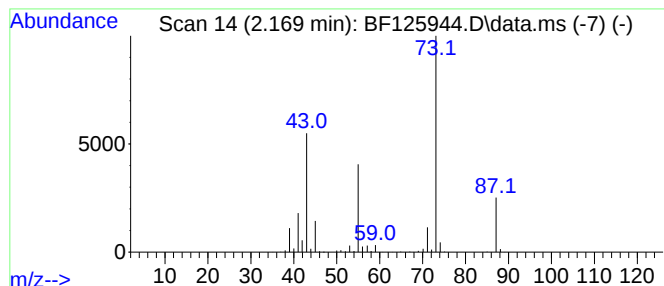
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.169	67.75 ng	3813770	1,4-Dichlorobenzene-d4	6.863

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-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
4			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35



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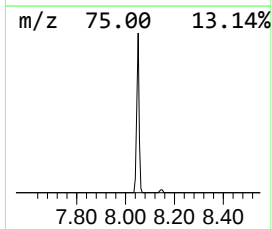
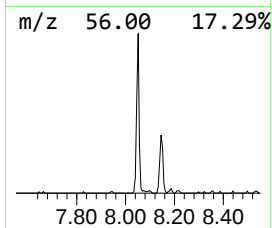
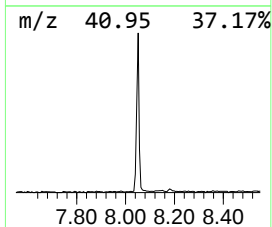
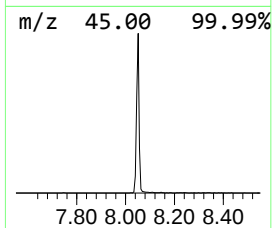
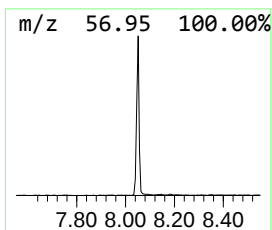
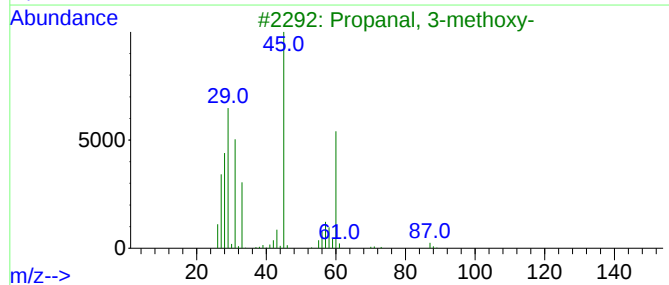
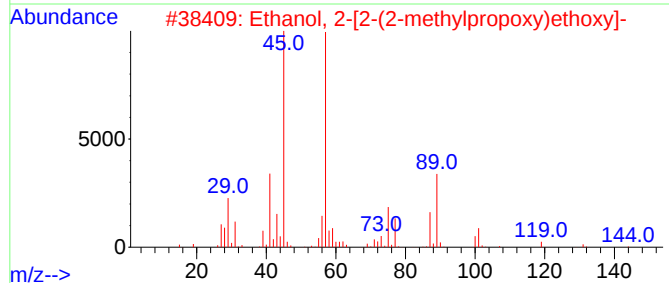
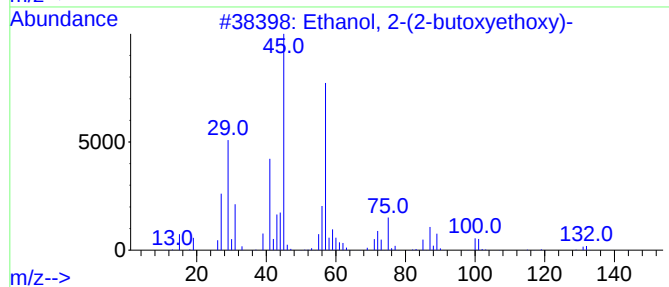
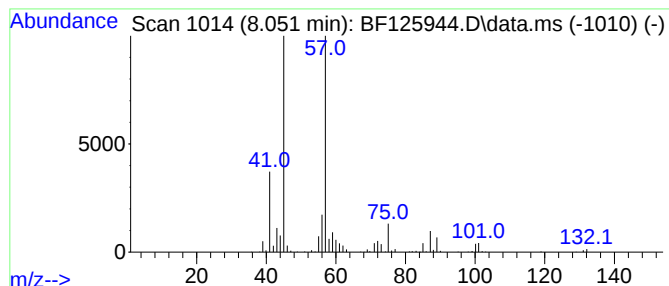
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	8.19 ng	587318	Naphthalene-d8	8.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Propanal, 3-methoxy-	88	C4H8O2	002806-84-0	50
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47



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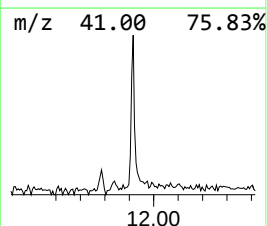
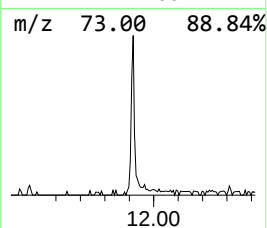
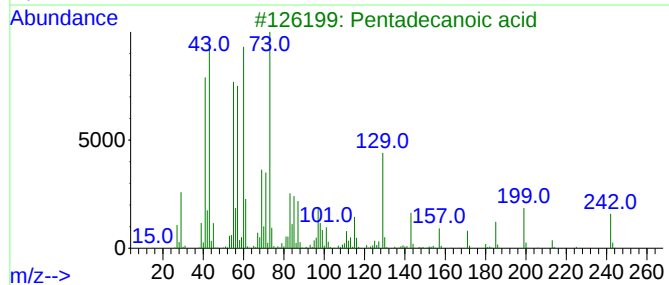
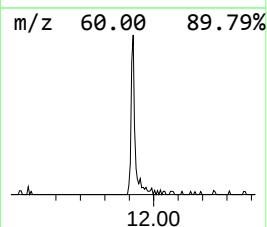
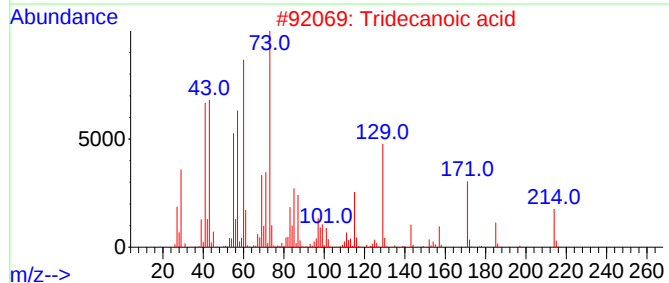
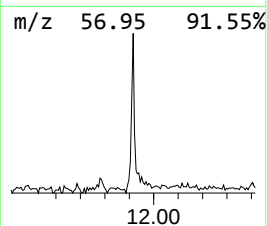
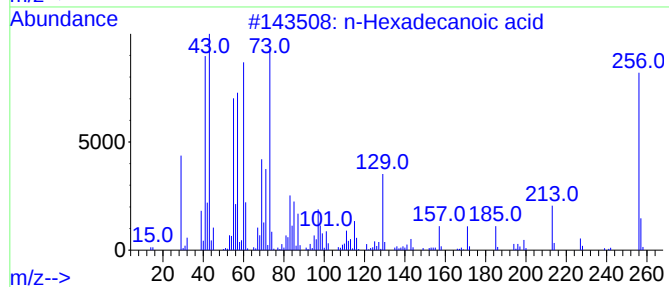
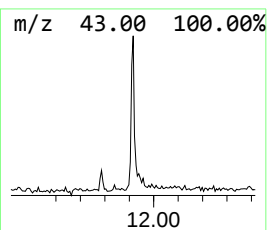
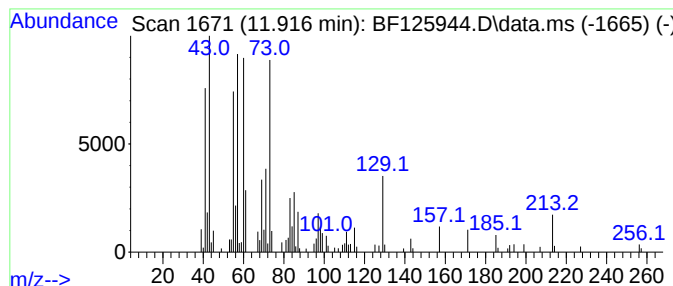
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.87 ng	220499	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	74



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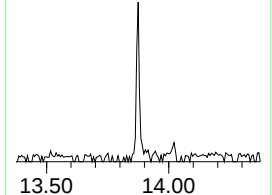
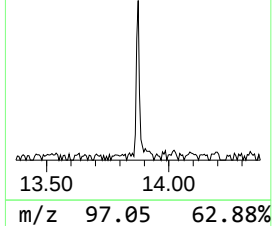
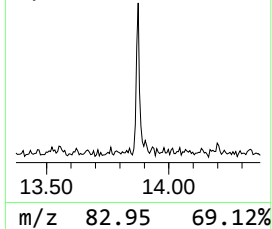
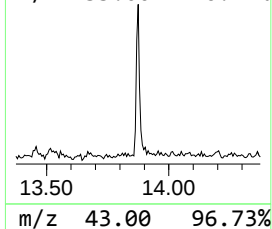
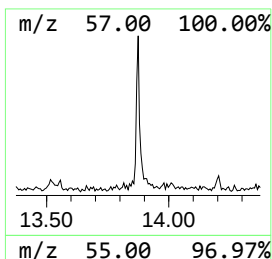
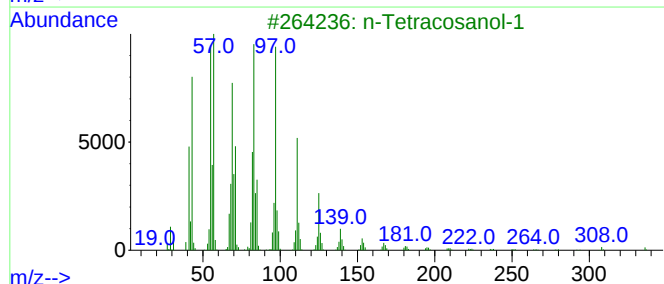
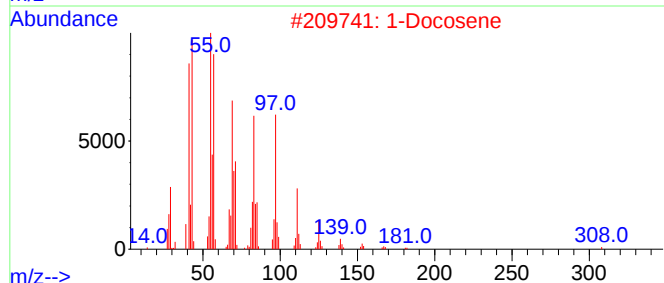
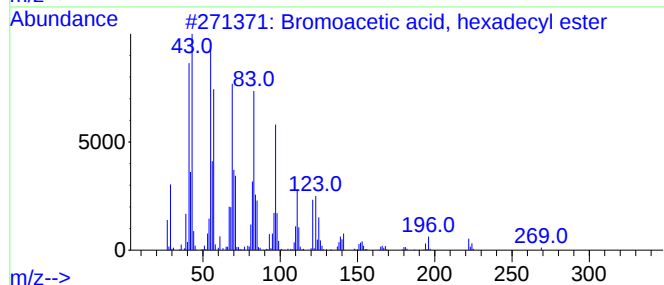
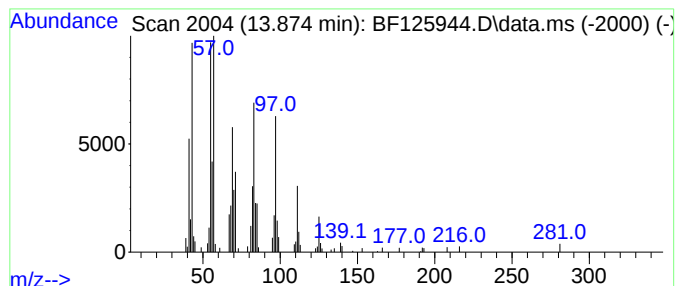
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Peak Number 4 Bromoacetic acid, hexadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.64 ng	162466	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
2			1-Docosene	308	C22H44	001599-67-3	91
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5			2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



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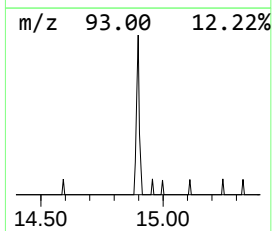
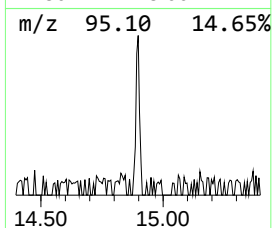
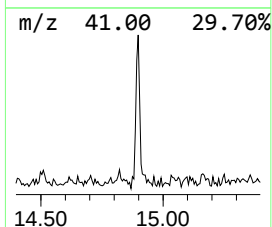
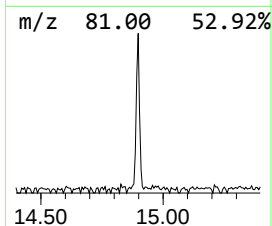
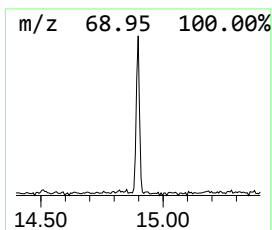
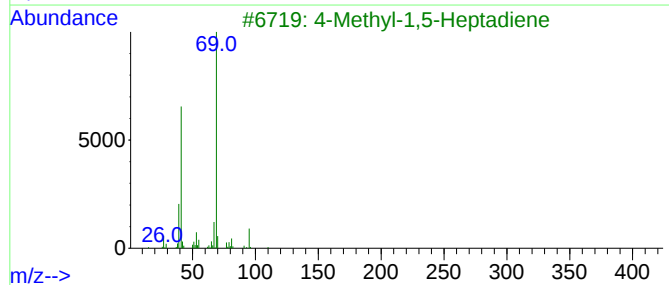
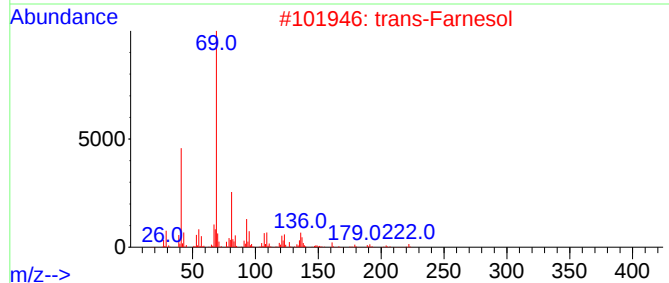
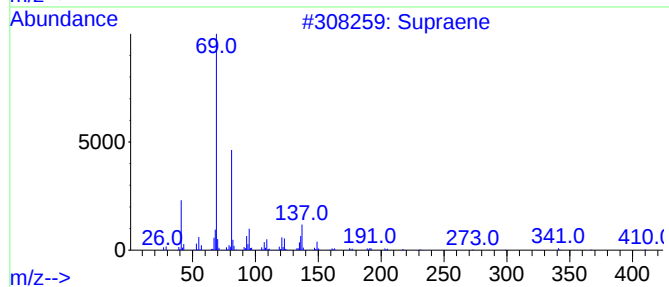
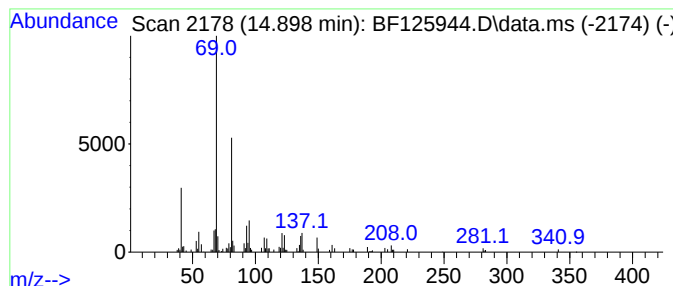
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.47 ng	117466	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			trans-Farnesol	222	C15H26O	000106-28-5	80
3			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	59
4			Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	59
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	67.8	ng	3813770	1	6.863	1125900	20.0
Ethanol, 2-(2-b...	8.051	8.2	ng	587318	2	8.145	1434070	20.0
n-Hexadecanoic ...	11.916	2.9	ng	220499	4	11.386	1536210	20.0
Bromoacetic aci...	13.874	3.6	ng	162466	5	14.021	893626	20.0
Supraene	14.898	2.5	ng	117466	6	15.492	949268	20.0