

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010722\
 Data File : BF126545.D
 Acq On : 7 Jan 2022 16:47
 Operator : JU/CG
 Sample : N1051-06
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-6-(4.5-5)

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126545.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.998	492	495	504	rVB	80278	95771	4.11%	0.555%
2	5.398	559	563	566	rBV	2168817	2192911	94.10%	12.705%
3	6.410	730	735	738	rBV	2086608	2271614	97.48%	13.161%
4	6.775	794	797	801	rBV	702637	621506	26.67%	3.601%
5	7.339	888	893	896	rBV	1443162	1494186	64.12%	8.657%
6	7.969	996	1000	1010	rBV	174544	198115	8.50%	1.148%
7	8.063	1011	1016	1019	rVV	834781	874090	37.51%	5.064%
8	9.139	1193	1199	1202	rBV	2319075	2330329	100.00%	13.501%
9	9.263	1216	1220	1225	rVB	41443	40215	1.73%	0.233%
10	9.816	1309	1314	1318	rBV	1038884	928984	39.86%	5.382%
11	10.604	1444	1448	1460	rVB	1336847	1378027	59.13%	7.984%
12	11.304	1563	1567	1570	rBV	1096498	889023	38.15%	5.151%
13	11.839	1655	1658	1667	rBV2	85761	111657	4.79%	0.647%
14	12.410	1746	1755	1763	rBV	42703	49695	2.13%	0.288%
15	12.627	1789	1792	1804	rBV2	24376	32954	1.41%	0.191%
16	12.898	1833	1838	1841	rBV	2129064	2035576	87.35%	11.793%
17	13.133	1873	1878	1890	rBV6	22983	61718	2.65%	0.358%
18	13.345	1905	1914	1917	rBV	55256	51538	2.21%	0.299%
19	13.821	1986	1995	2011	rBV5	60125	194838	8.36%	1.129%
20	13.951	2013	2017	2021	rVB	683630	621896	26.69%	3.603%
21	14.445	2097	2101	2105	rBV	28729	26336	1.13%	0.153%
22	14.757	2150	2154	2157	rVB	30502	31651	1.36%	0.183%
23	15.086	2205	2210	2214	rBV	37826	40494	1.74%	0.235%
24	15.415	2261	2266	2270	rBV	427482	519572	22.30%	3.010%
25	15.456	2270	2273	2278	rVB	39125	50466	2.17%	0.292%
26	15.886	2340	2346	2354	rBV	33883	50829	2.18%	0.294%
27	16.380	2424	2430	2437	rVB2	22906	42004	1.80%	0.243%
28	17.633	2638	2643	2652	rBV5	10305	24276	1.04%	0.141%

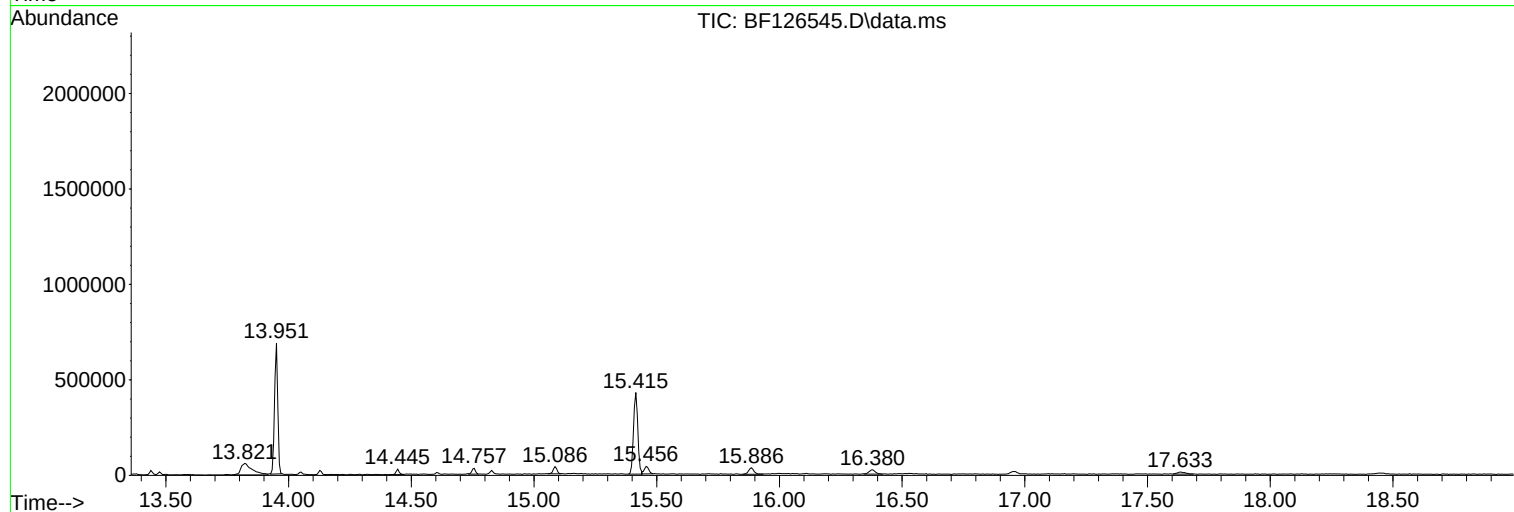
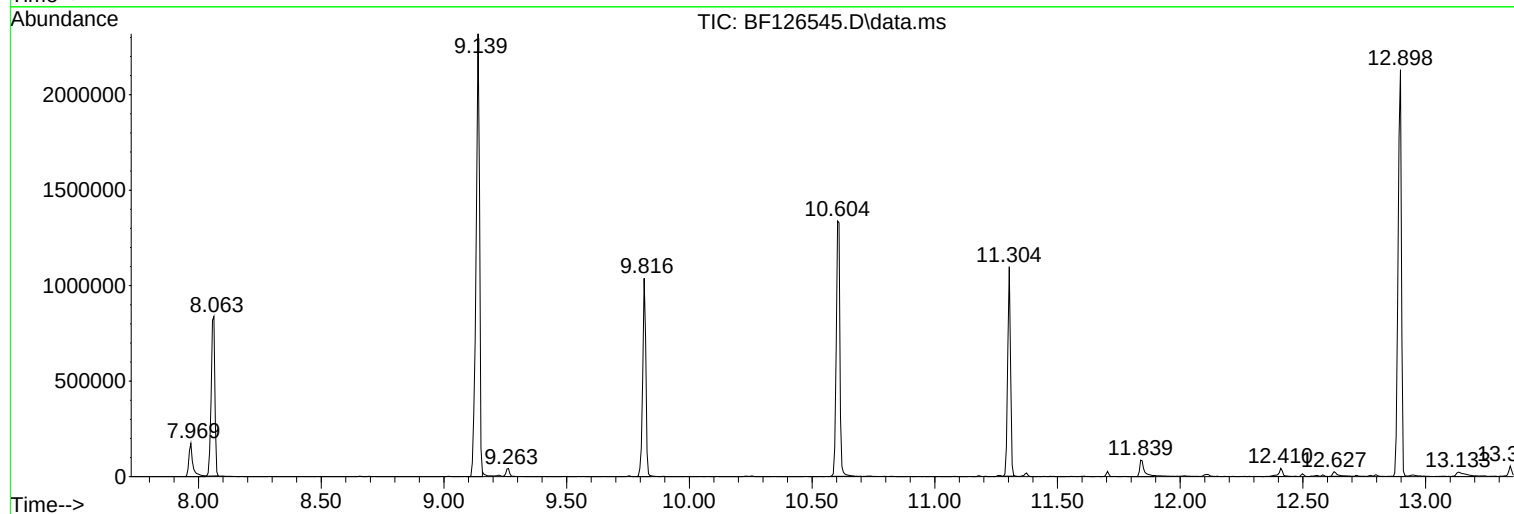
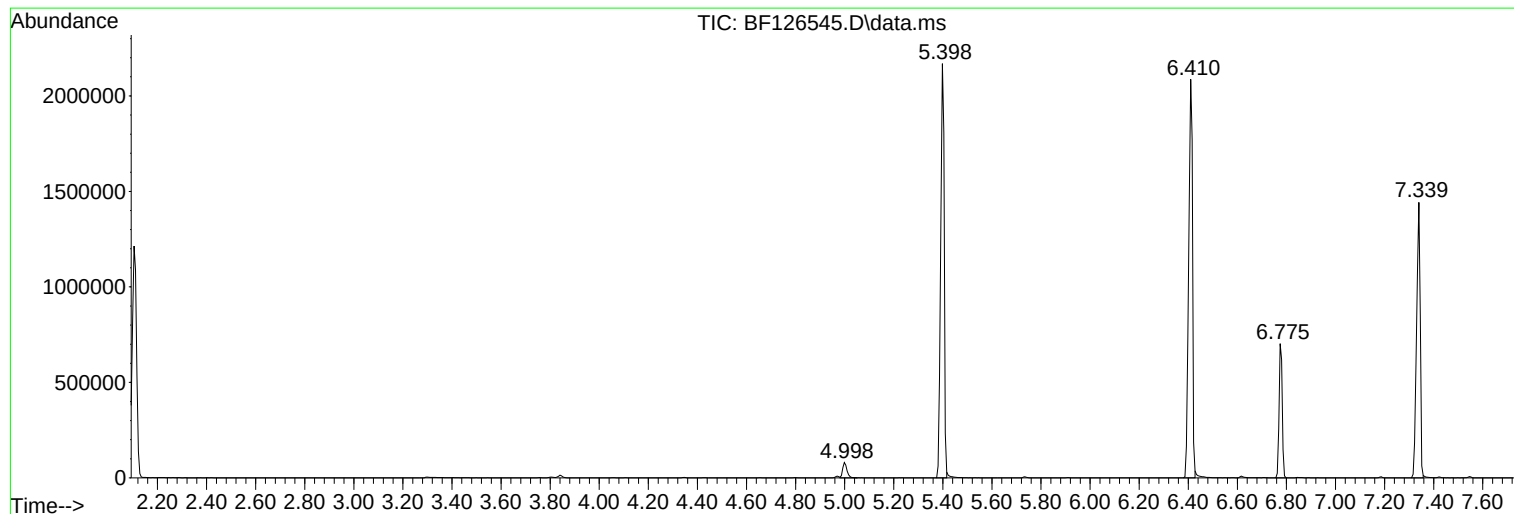
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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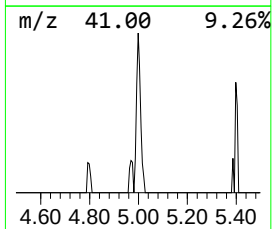
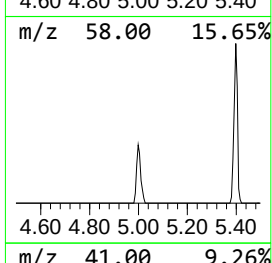
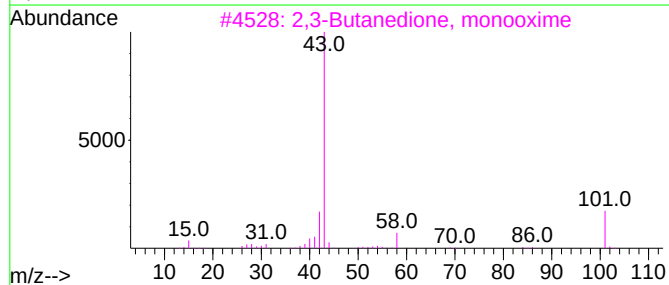
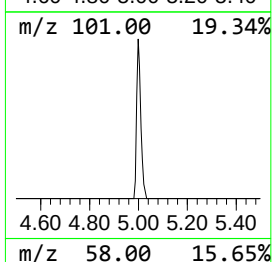
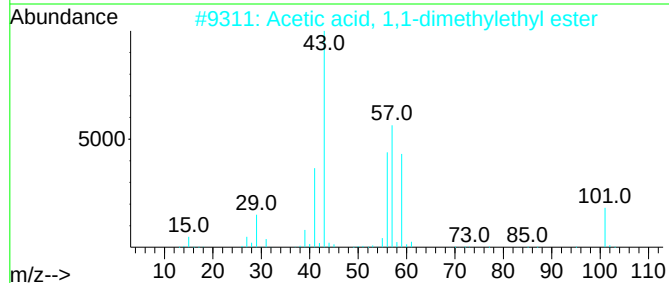
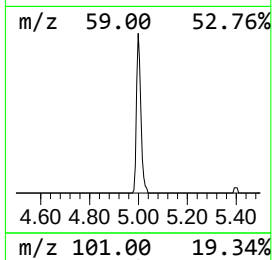
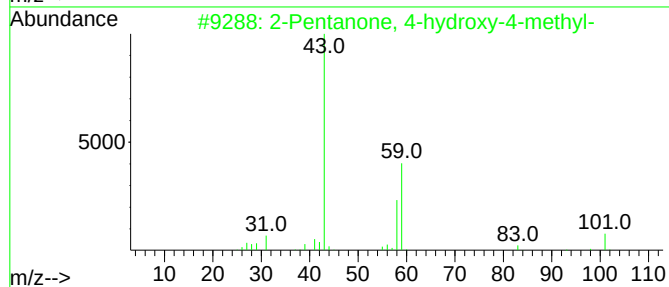
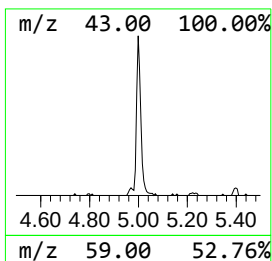
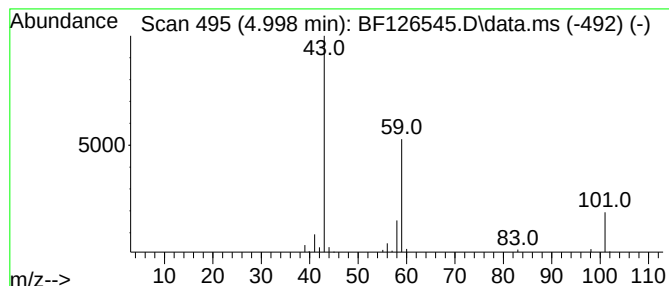
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	3.08 ng	95771	1,4-Dichlorobenzene-d4	6.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32		
4	1,2-Butanediol	90	C4H10O2	000584-03-2	23		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		



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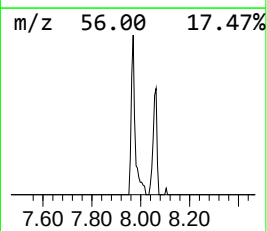
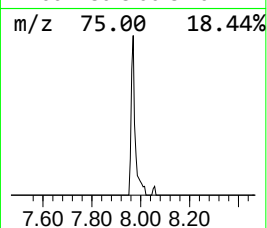
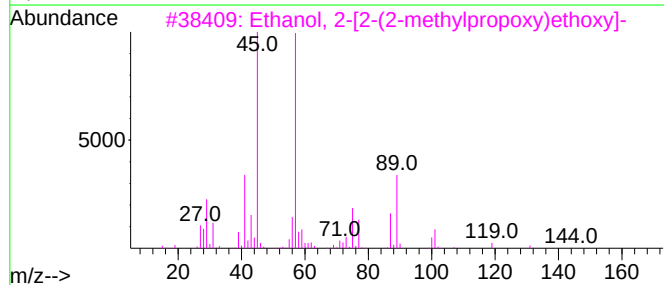
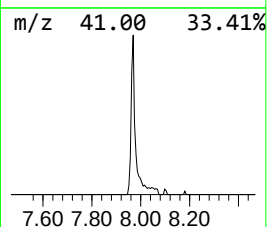
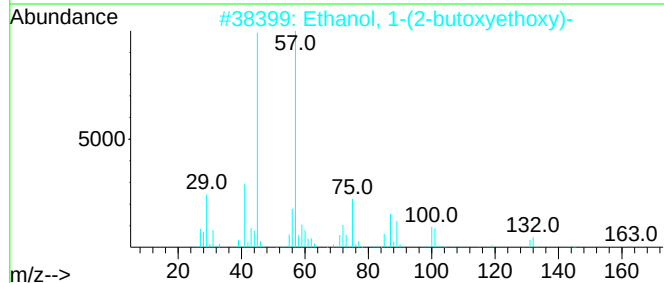
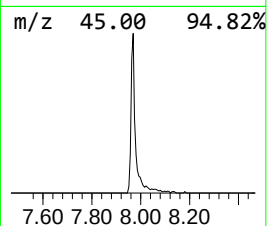
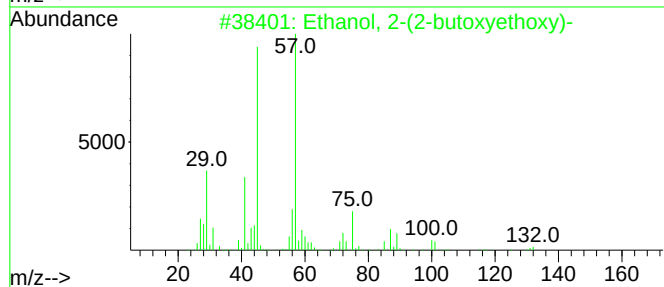
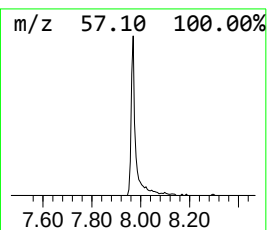
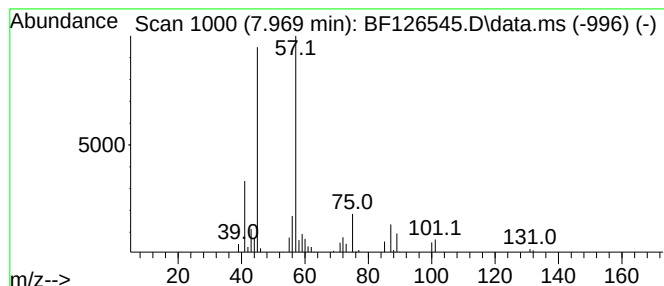
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.969	4.53 ng	198115	Naphthalene-d8	8.063

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	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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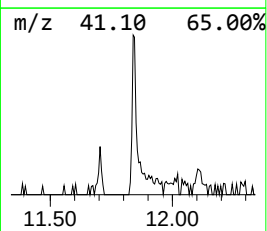
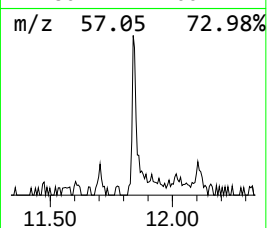
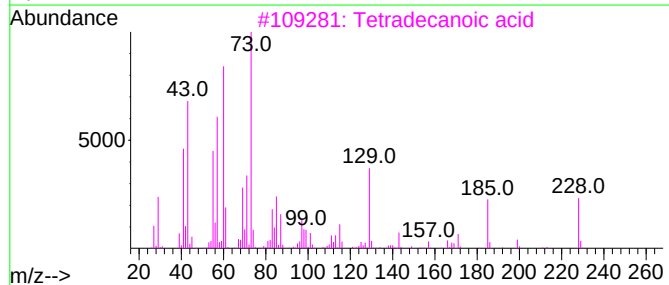
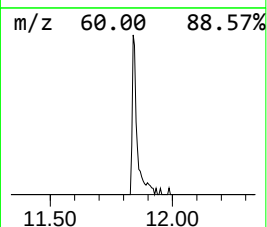
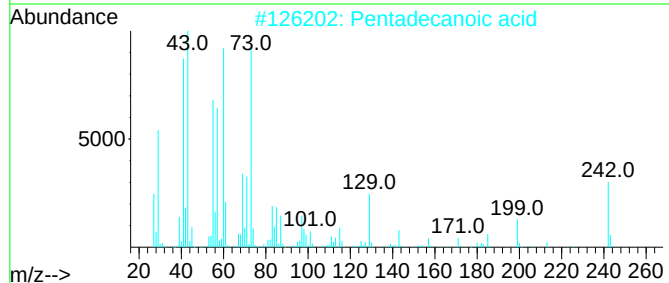
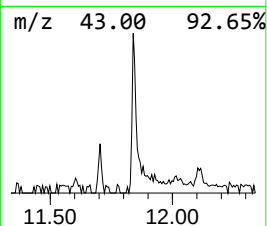
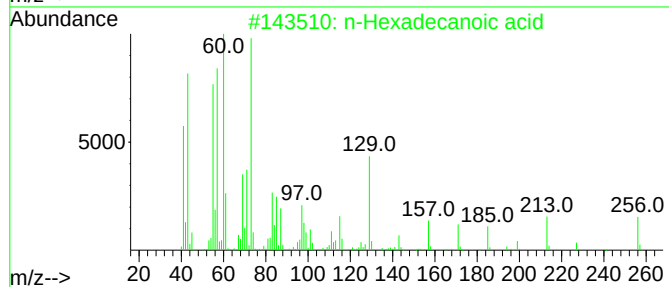
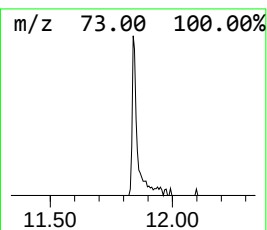
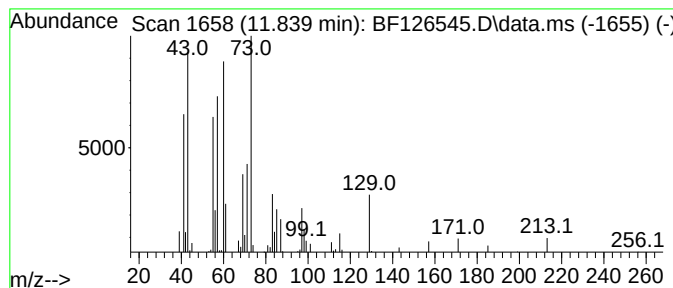
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	2.51 ng	111657	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Undecanoic acid	186	C11H22O2	000112-37-8	64
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	18



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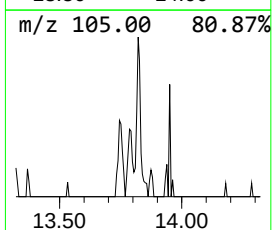
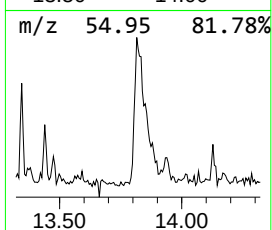
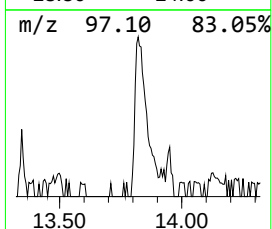
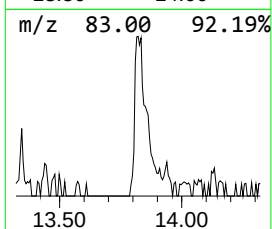
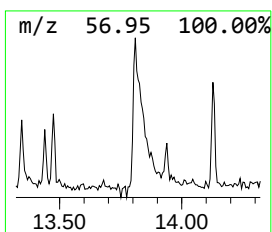
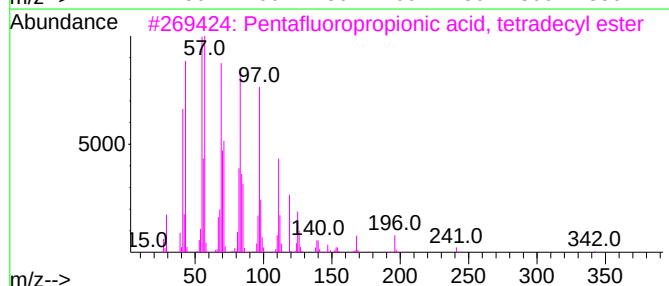
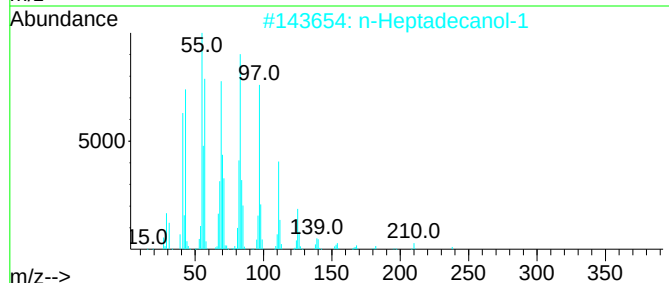
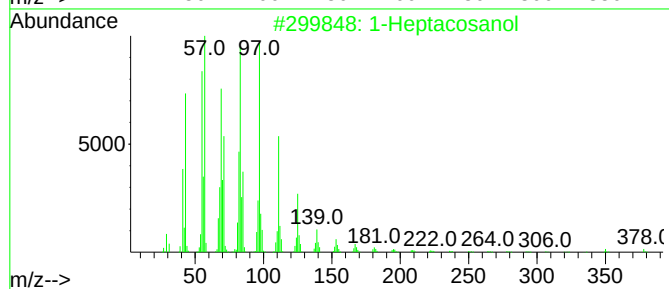
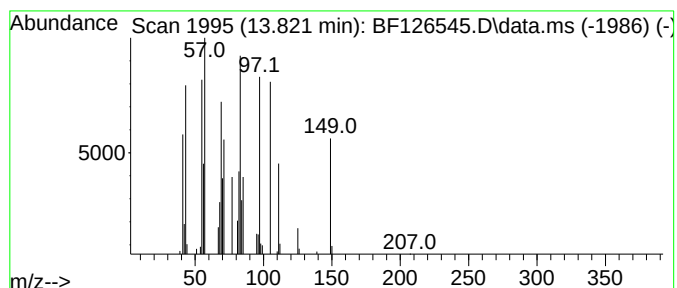
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Peak Number 4 1-Heptacosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	6.27 ng	194838	Chrysene-d12	13.951

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	74
2		n-Heptadecanol-1	256	C17H36O	001454-85-9	70
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	68
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	68
5		1-Tricosene	322	C23H46	018835-32-0	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.998	3.1	ng	95771	1	6.775	621506	20.0
Ethanol, 2-(2-b...	7.969	4.5	ng	198115	2	8.063	874090	20.0
n-Hexadecanoic ...	11.839	2.5	ng	111657	4	11.304	889023	20.0
1-Heptacosanol	13.821	6.3	ng	194838	5	13.951	621896	20.0