

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
 Data File : BF126070.D
 Acq On : 8 Nov 2021 17:48
 Operator : JU/CG
 Sample : M4540-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126070.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	20	rBV	2314176	3032554	51.92%	7.796%
2	5.087	506	510	516	rVB	130205	168774	2.89%	0.434%
3	5.475	571	576	579	rBV	5278488	5387166	92.24%	13.849%
4	6.481	741	747	750	rBV	4650237	5520932	94.53%	14.193%
5	6.851	807	810	814	rBV	1298643	1013144	17.35%	2.604%
6	7.416	900	906	909	rBV	3766116	3507266	60.05%	9.016%
7	8.039	1007	1012	1024	rBV	1461770	1339916	22.94%	3.444%
8	8.133	1024	1028	1032	rVB	1502560	1190293	20.38%	3.060%
9	9.210	1206	1211	1214	rBV	6723045	5840666	100.00%	15.014%
10	9.886	1322	1326	1336	rBV	1499618	1202093	20.58%	3.090%
11	10.674	1456	1460	1463	rBV	3472691	2894052	49.55%	7.440%
12	11.368	1574	1578	1586	rBV	1161290	1006648	17.24%	2.588%
13	11.768	1642	1646	1650	rVB	101292	82594	1.41%	0.212%
14	12.957	1844	1848	1851	rBV	5541716	4435454	75.94%	11.402%
15	13.386	1918	1921	1925	rBV	101020	86944	1.49%	0.224%
16	13.498	1936	1940	1943	rBV	88905	87651	1.50%	0.225%
17	13.862	1998	2002	2012	rBV2	185348	314821	5.39%	0.809%
18	14.004	2022	2026	2030	rBV	990500	939540	16.09%	2.415%
19	15.468	2270	2275	2281	rBV	586817	767535	13.14%	1.973%
20	17.056	2540	2545	2551	rVB7	41312	82209	1.41%	0.211%

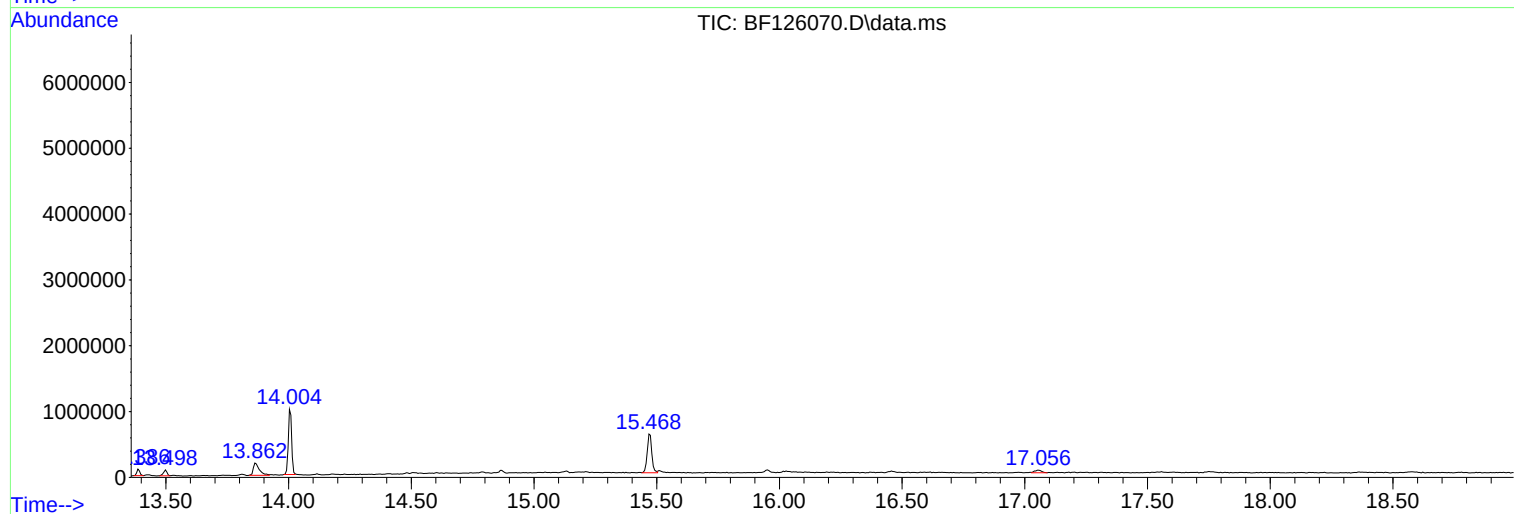
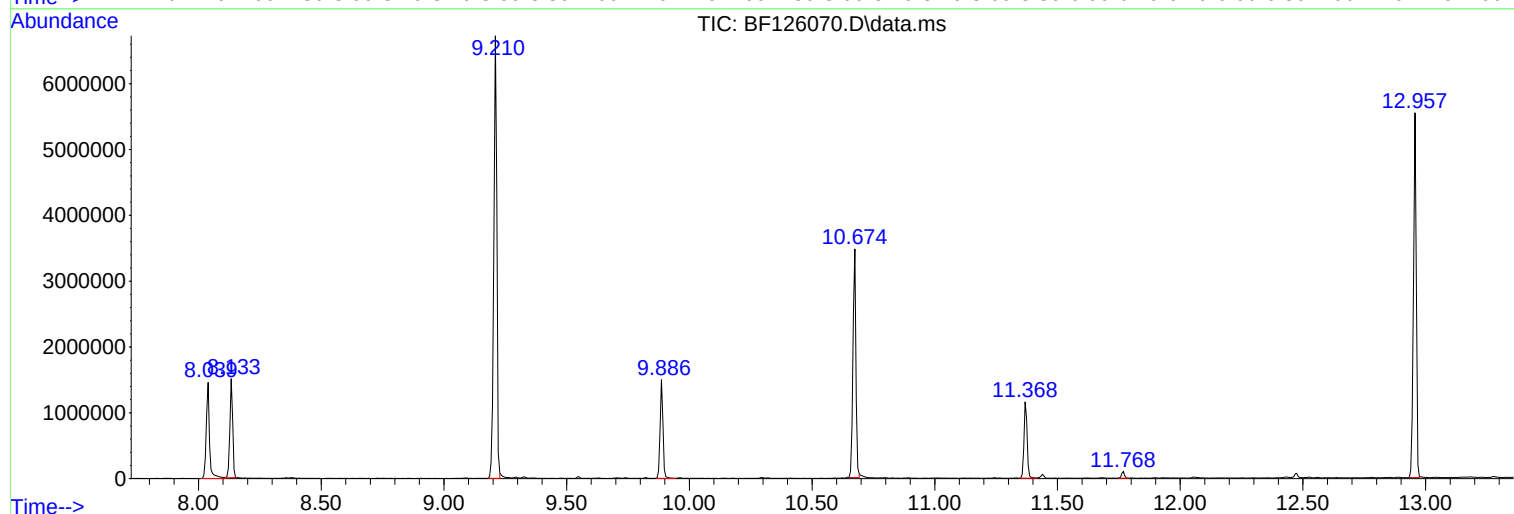
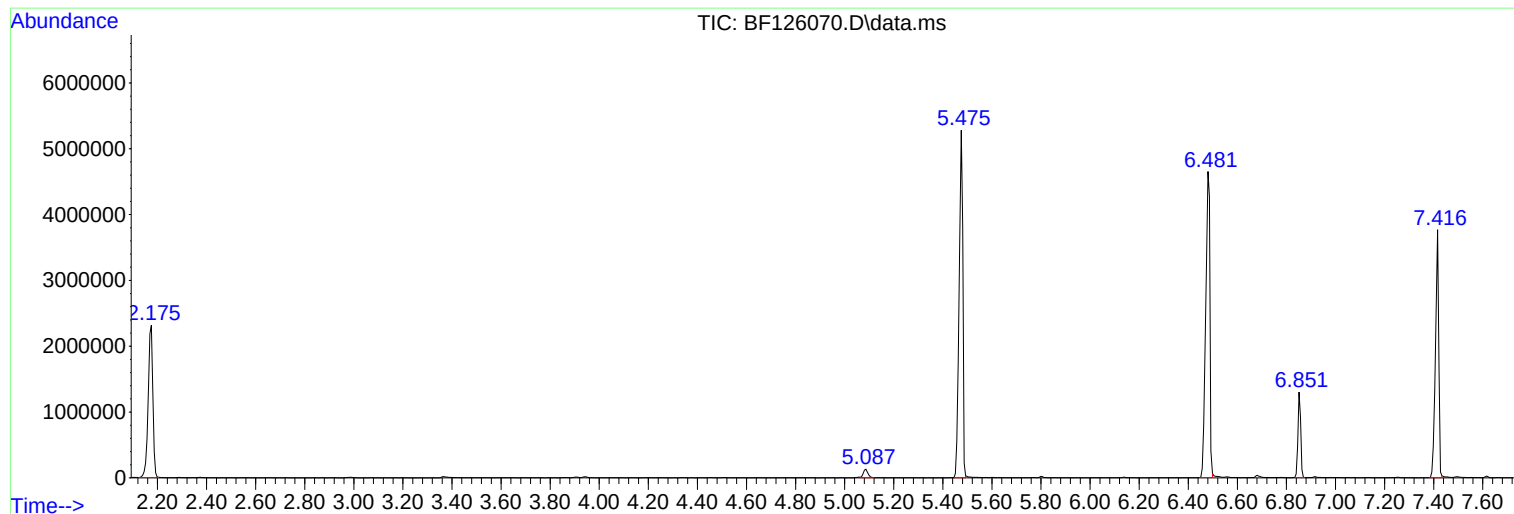
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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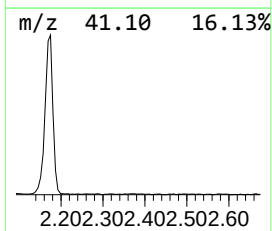
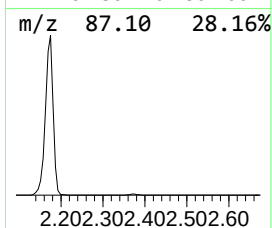
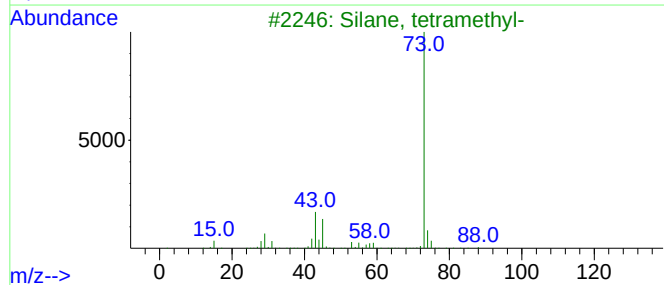
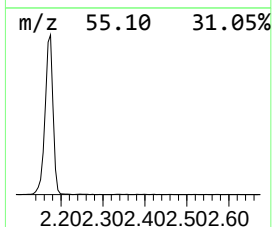
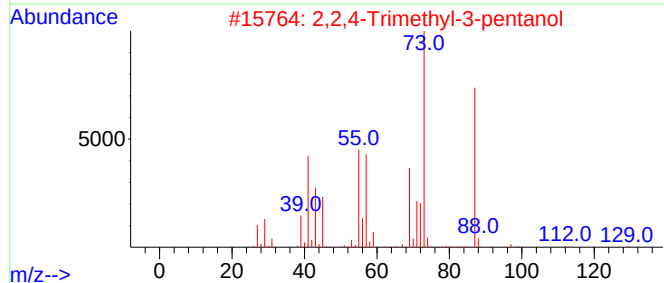
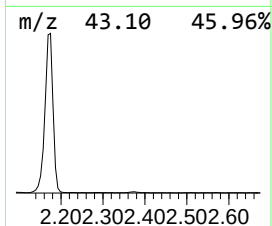
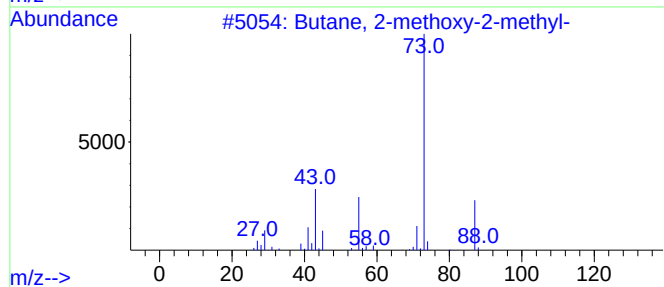
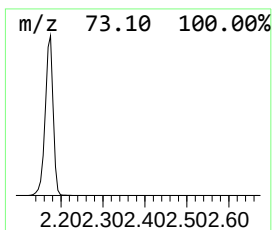
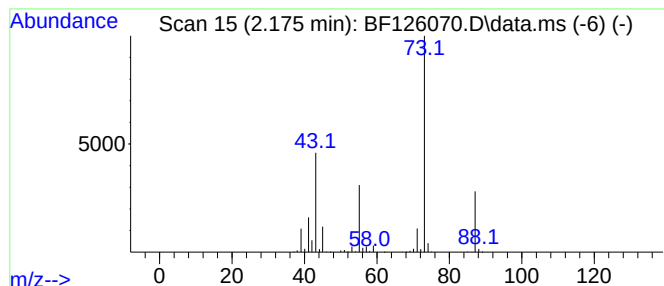
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	59.86 ng	3032550	1,4-Dichlorobenzene-d4	6.851

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	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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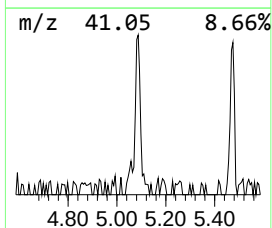
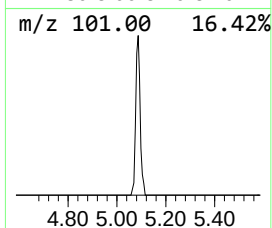
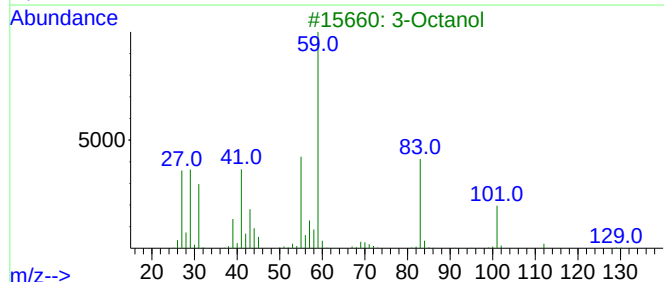
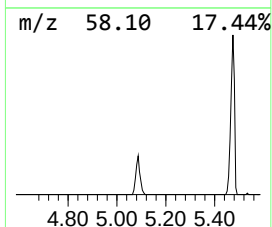
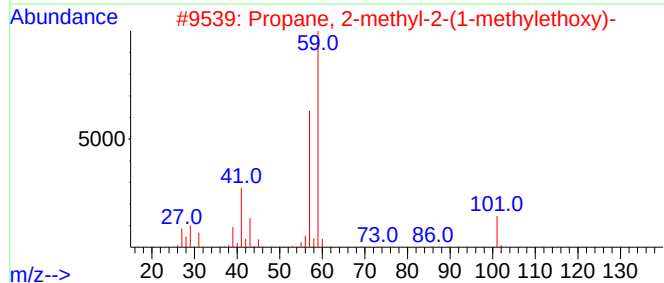
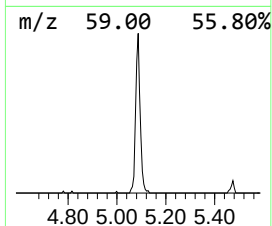
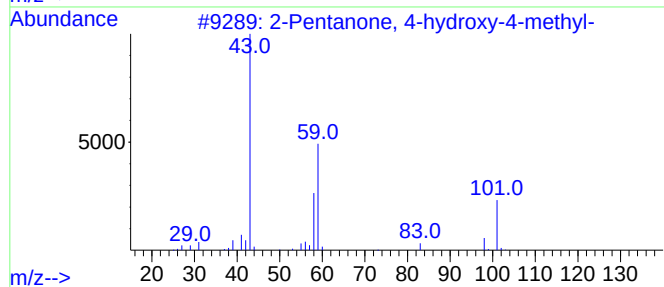
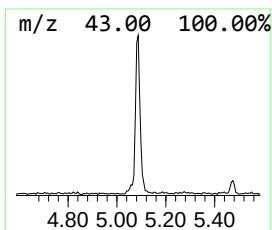
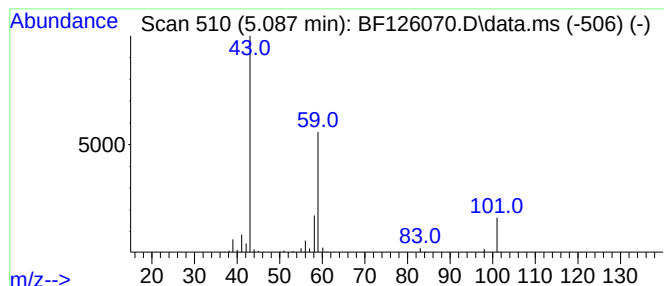
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	3.33 ng	168774	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Octanol	130	C8H18O	000589-98-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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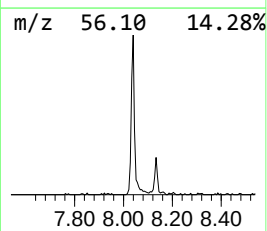
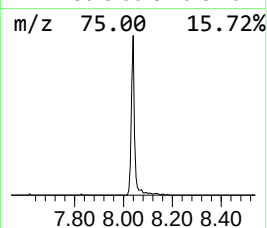
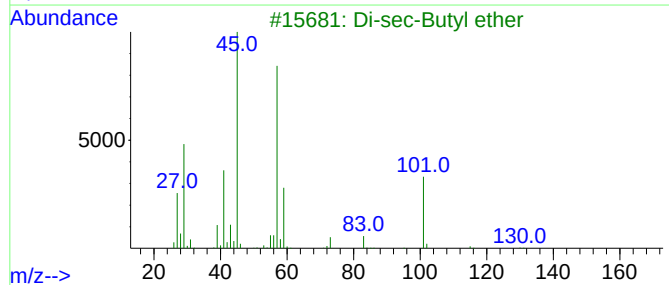
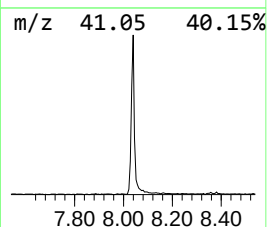
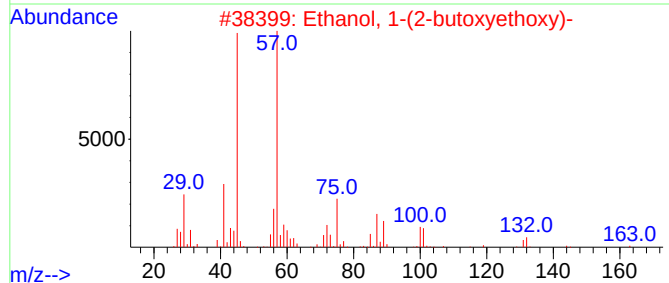
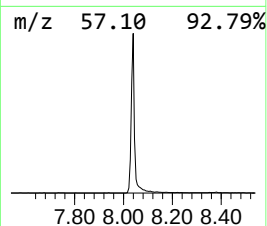
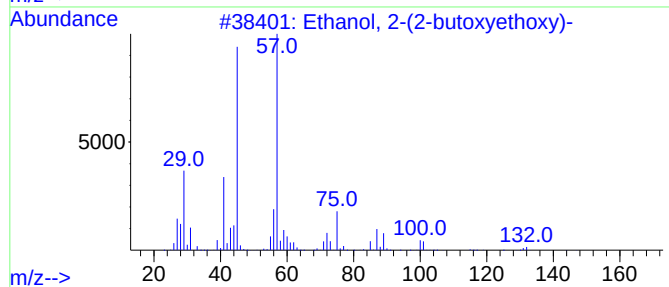
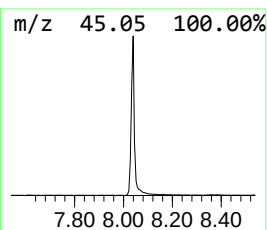
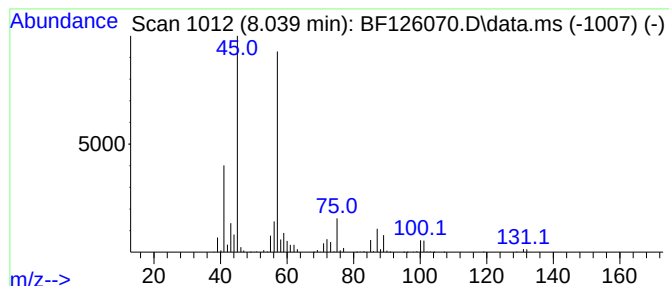
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	22.51 ng	1339920	Naphthalene-d8	8.133

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			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Butyl lactate	146	C7H14O3	000138-22-7	50



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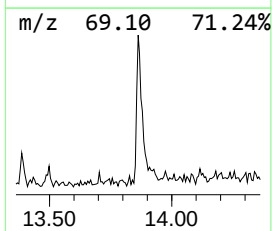
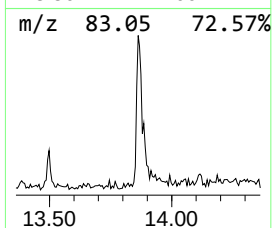
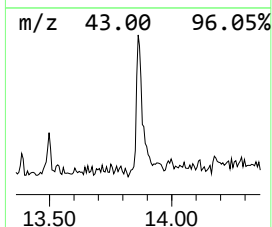
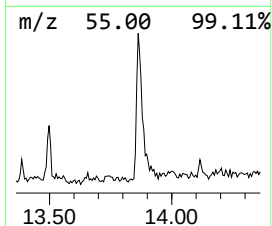
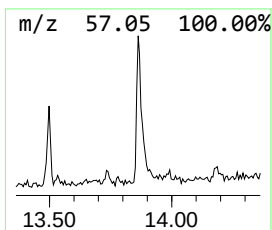
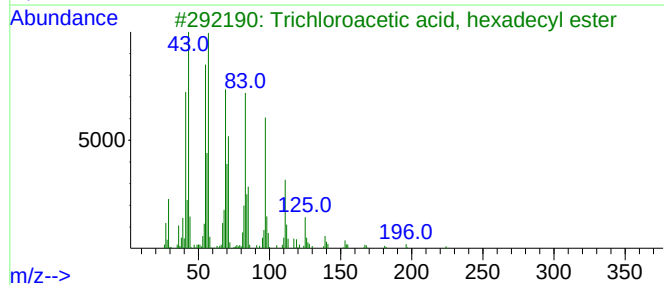
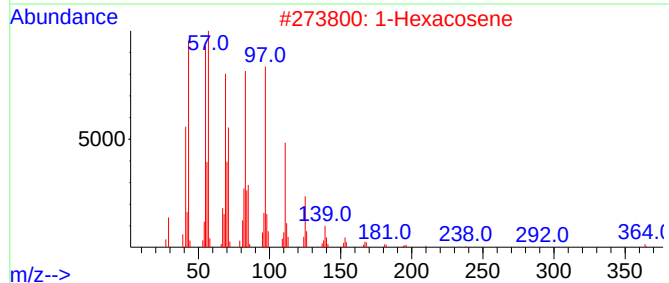
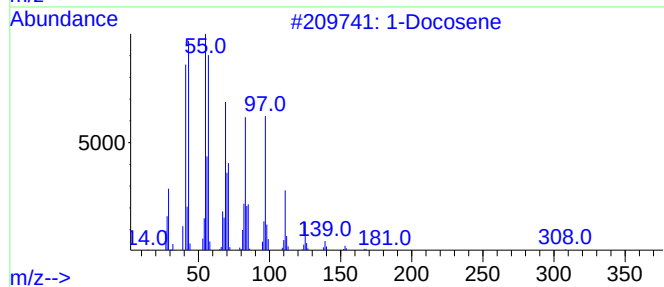
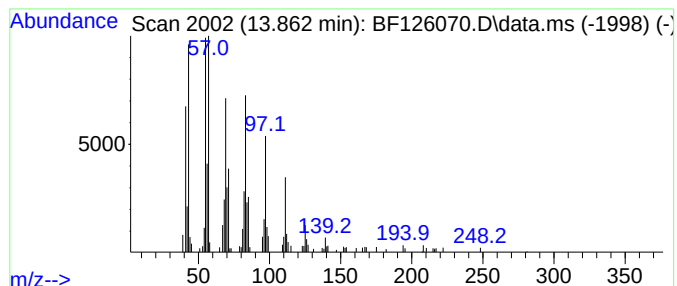
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Peak Number 4 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	6.70 ng	314821	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	1-Hexacosene			364	C26H52	018835-33-1	91
3	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	91
4	n-Tetracosanol-1			354	C24H50O	000506-51-4	91
5	Behenic alcohol			326	C22H46O	000661-19-8	91



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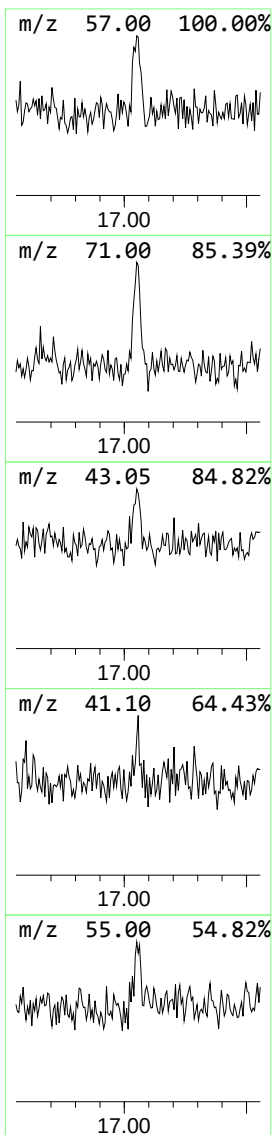
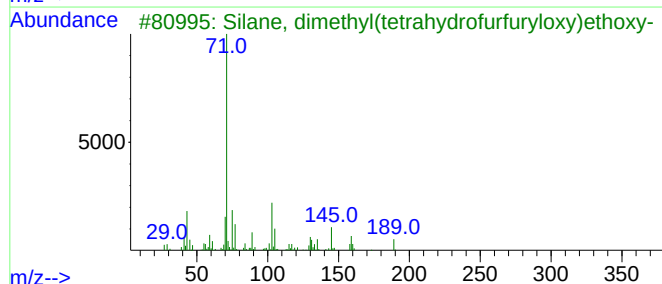
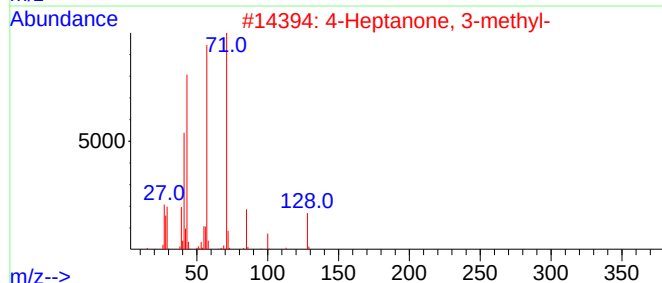
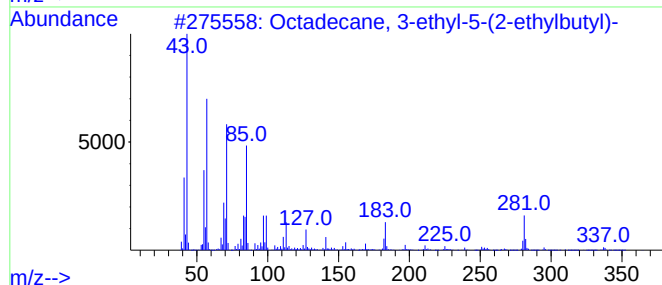
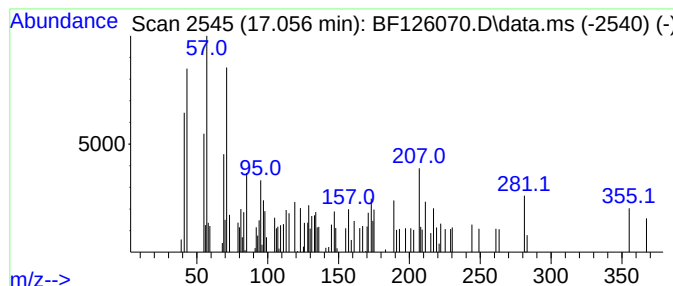
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Peak Number 5 unknown17.056 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.056	2.14 ng	82209	Perylene-d12	15.468	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	35
2	4-Heptanone, 3-methyl-	128	C8H16O	015726-15-5	25
3	Silane, dimethyl(tetrahydrofurfu...	204	C9H20O3Si	1000347-82-4	22
4	Decane, 5-ethyl-5-methyl-	184	C13H28	017312-74-2	22
5	1,2,5-Triazole 2-oxide, 1-sec-bu...	201	C6H11N5O3	339589-40-1	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	59.9	ng	3032550	1	6.851	1013140	20.0
2-Pentanone, 4-...	5.087	3.3	ng	168774	1	6.851	1013140	20.0
Ethanol, 2-(2-b...	8.039	22.5	ng	1339920	2	8.133	1190290	20.0
1-Docosene	13.863	6.7	ng	314821	5	14.004	939540	20.0
unknown17.056	17.056	2.1	ng	82209	6	15.468	767535	20.0