

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
 Data File : BF125191.D
 Acq On : 24 Aug 2021 18:24
 Operator : JU/CG
 Sample : M3521-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 124019

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: BF125191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	14	19	26	rVB	811446	1067114	42.74%	4.690%
2	5.528	581	585	588	rBV	2721722	2469264	98.90%	10.854%
3	6.534	751	756	759	rBV	2708903	2462155	98.61%	10.822%
4	6.916	817	821	824	rBV	943845	778023	31.16%	3.420%
5	7.475	911	916	919	rBV	1891629	1594202	63.85%	7.007%
6	8.092	1018	1021	1035	rBV	159043	239401	9.59%	1.052%
7	8.198	1035	1039	1041	rVV	1231062	1021580	40.92%	4.490%
8	8.216	1041	1042	1046	rVB	106993	72706	2.91%	0.320%
9	9.269	1217	1221	1224	rBV	3098198	2496757	100.00%	10.974%
10	9.380	1236	1240	1244	rBV2	32252	31217	1.25%	0.137%
11	9.951	1333	1337	1340	rBV	1396208	1104500	44.24%	4.855%
12	9.980	1340	1342	1346	rVB	112845	89879	3.60%	0.395%
13	10.157	1366	1372	1376	rBV	41620	37763	1.51%	0.166%
14	10.498	1426	1430	1433	rBV	62251	48586	1.95%	0.214%
15	10.739	1467	1471	1474	rBV	1959168	1764020	70.65%	7.754%
16	11.439	1586	1590	1592	rBV	1246059	1103204	44.19%	4.849%
17	11.463	1592	1594	1597	rVV	354097	273773	10.97%	1.203%
18	11.510	1600	1602	1605	rVB	47721	41774	1.67%	0.184%
19	11.951	1672	1677	1683	rBV3	122970	175656	7.04%	0.772%
20	12.051	1691	1694	1696	rBV2	57072	56144	2.25%	0.247%
21	12.533	1770	1776	1780	rVV2	93323	86493	3.46%	0.380%
22	12.574	1780	1783	1787	rVB	32349	31851	1.28%	0.140%
23	12.651	1793	1796	1799	rVB	488344	378450	15.16%	1.663%
24	12.739	1809	1811	1815	rBV2	37156	34505	1.38%	0.152%
25	12.880	1829	1835	1838	rBV	377183	366683	14.69%	1.612%
26	13.021	1855	1859	1862	rBV	2566653	2100820	84.14%	9.234%
27	13.204	1888	1890	1893	rVB	30807	29829	1.19%	0.131%
28	13.945	2013	2016	2018	rBV	53057	48554	1.94%	0.213%
29	14.080	2031	2039	2041	rBV	981022	1069498	42.84%	4.701%
30	14.104	2041	2043	2048	rVB	163590	143447	5.75%	0.631%
31	15.133	2213	2218	2221	rBV	109811	184853	7.40%	0.813%
32	15.445	2267	2271	2276	rVB	61130	77430	3.10%	0.340%
33	15.504	2277	2281	2286	rVV	65775	81502	3.26%	0.358%
34	15.574	2288	2293	2306	rBV2	812150	1062289	42.55%	4.669%
35	16.051	2371	2374	2381	rVB6	20681	32092	1.29%	0.141%
36	17.074	2543	2548	2556	rVB2	29281	60829	2.44%	0.267%

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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

37	17.527	2623	2625	2632	rVB5	22734	33715	1.35%	0.148%
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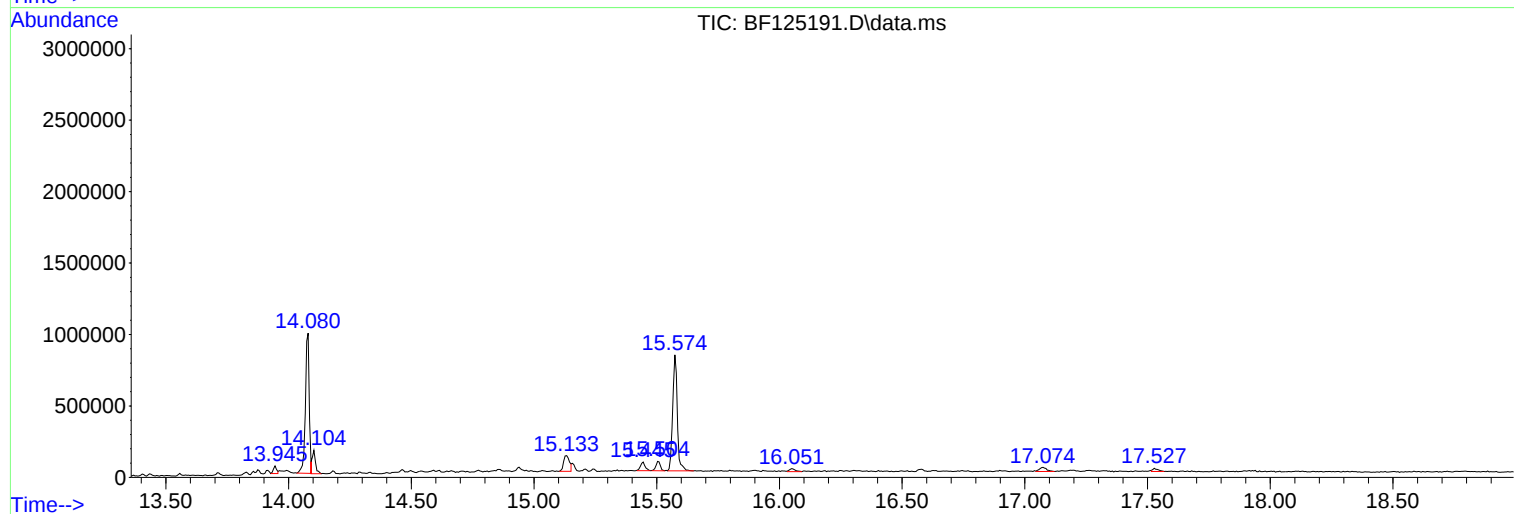
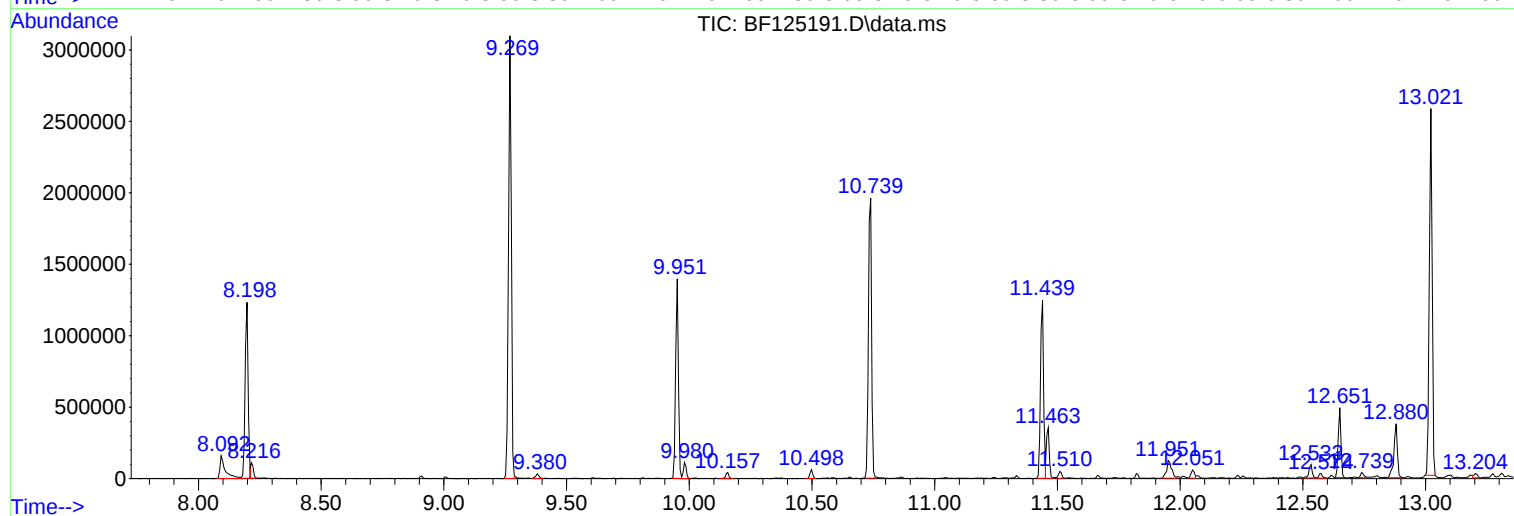
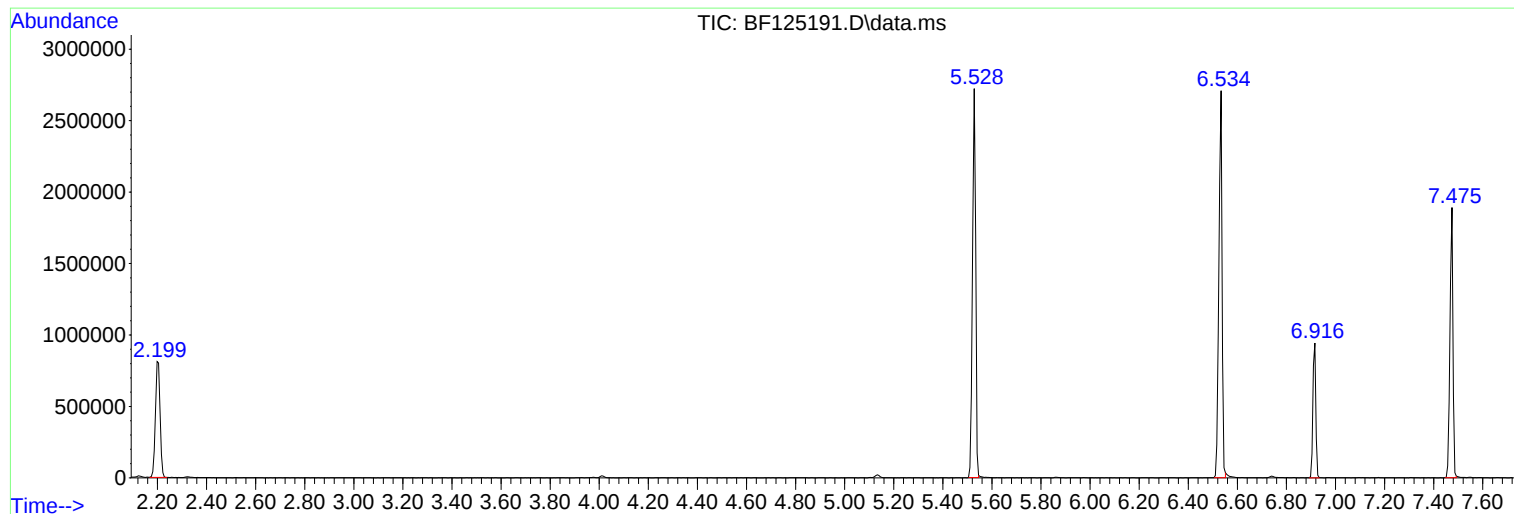
Sum of corrected areas: 22750558

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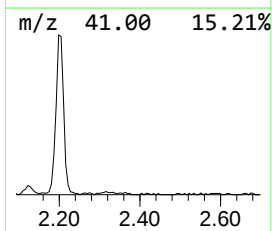
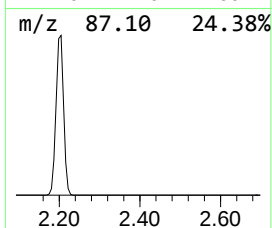
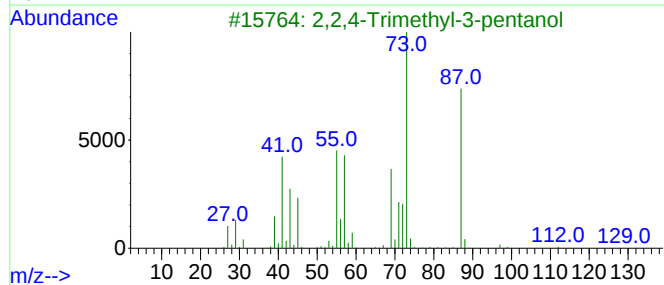
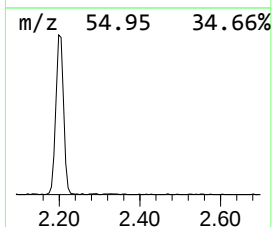
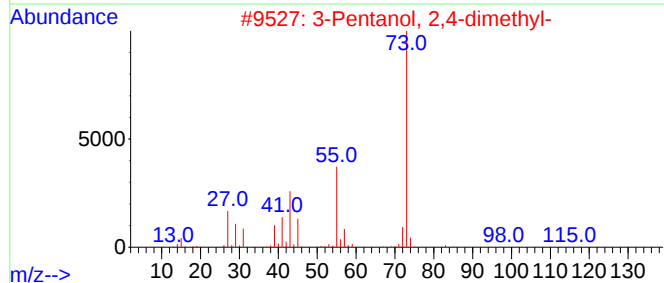
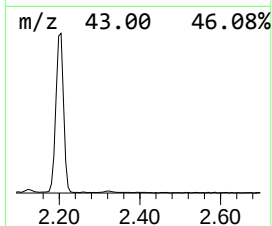
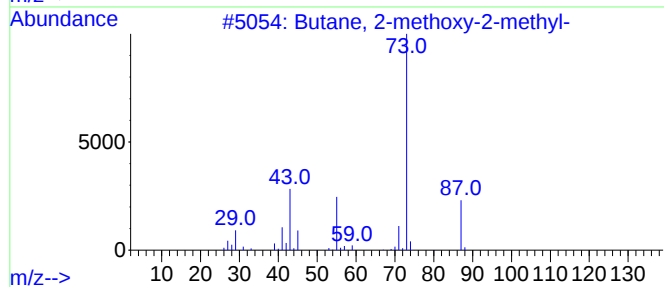
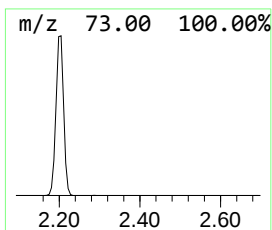
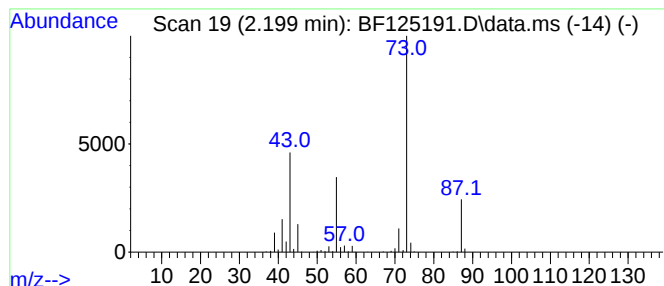
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	27.43 ng	1067110	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	39
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23



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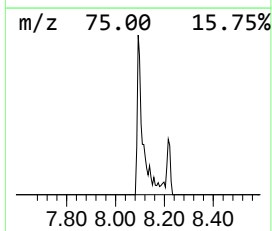
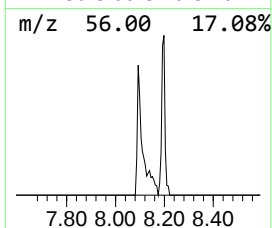
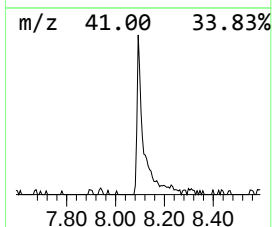
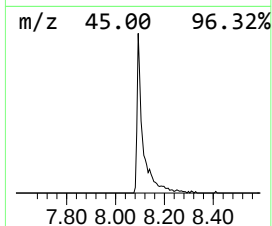
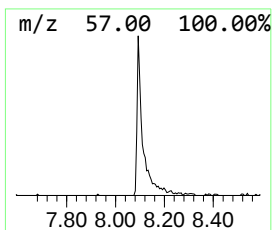
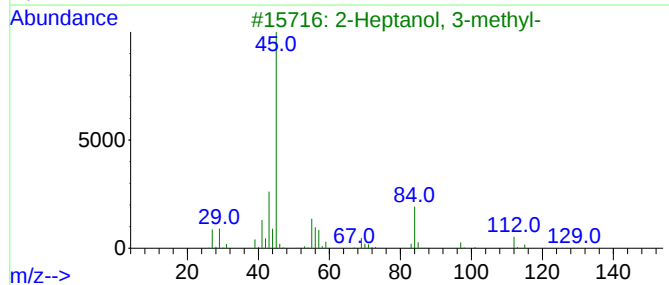
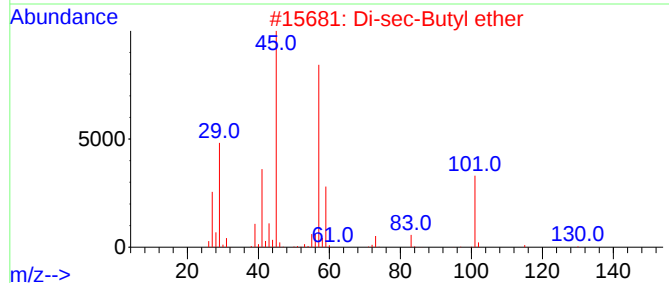
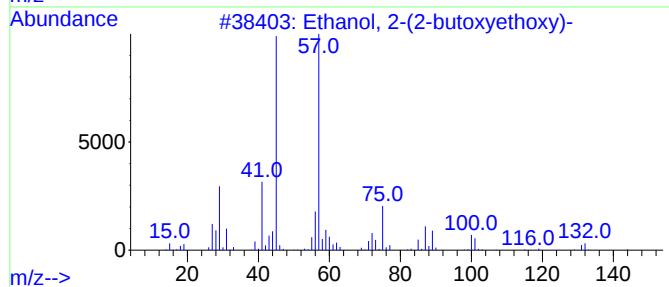
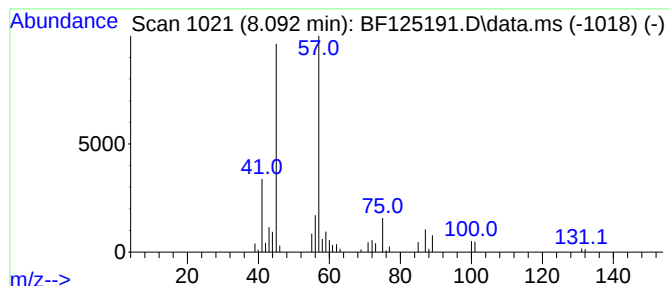
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	4.69 ng	239401	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			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
3			2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	50
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	50



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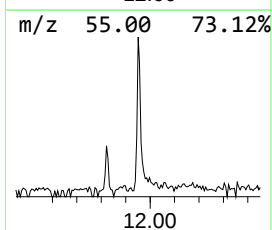
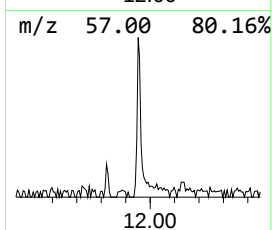
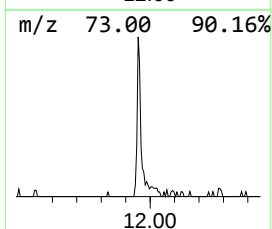
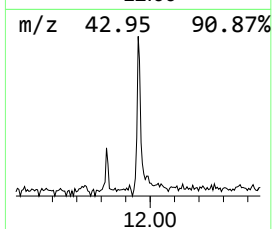
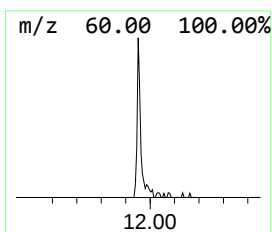
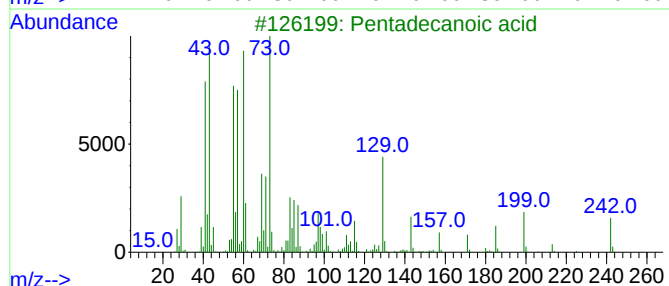
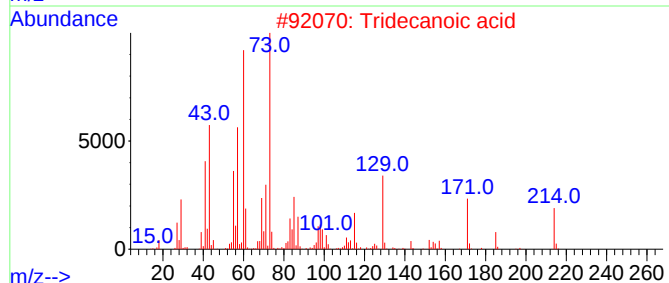
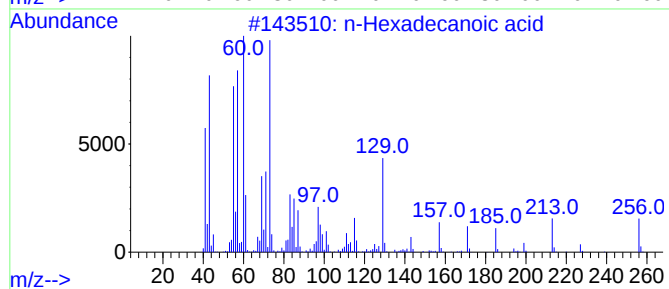
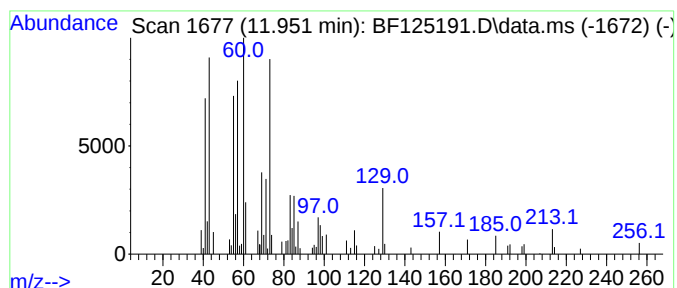
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.951	3.18 ng	175656	Phenanthrene-d10	11.439	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72



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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...	2.199	27.4	ng	1067110	1	6.916	778023	20.0
Ethanol, 2-(2-b...	8.092	4.7	ng	239401	2	8.198	1021580	20.0
n-Hexadecanoic ...	11.951	3.2	ng	175656	4	11.439	1103200	20.0