

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100523\
 Data File : BF135603.D
 Acq On : 05 Oct 2023 17:03
 Operator : CG\JU
 Sample : 04712-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-1

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135603.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	485	489	508	rBV	1102506	1563188	46.31%	6.367%
2	5.381	556	560	582	rBV	3035316	3375471	100.00%	13.748%
3	5.763	621	625	631	rBV	37849	42671	1.26%	0.174%
4	6.393	728	732	753	rBV	3231643	3278960	97.14%	13.355%
5	6.581	761	764	777	rBV	90350	120356	3.57%	0.490%
6	6.740	787	791	799	rVB	884719	737335	21.84%	3.003%
7	7.281	880	883	884	rBV	168919	133097	3.94%	0.542%
8	7.304	884	887	890	rVB	2113626	2001238	59.29%	8.151%
9	8.016	1005	1008	1026	rVB	1152673	955269	28.30%	3.891%
10	9.098	1187	1192	1195	rBV	3459151	3311159	98.09%	13.486%
11	9.210	1208	1211	1216	rVB	106506	103341	3.06%	0.421%
12	9.775	1303	1307	1310	rBV	1045481	971056	28.77%	3.955%
13	10.569	1438	1442	1451	rBV	2054433	1856612	55.00%	7.562%
14	11.263	1557	1560	1563	rBV	950284	901455	26.71%	3.672%
15	11.292	1563	1565	1569	rVV	130887	114630	3.40%	0.467%
16	11.345	1569	1574	1578	rVB	29487	38700	1.15%	0.158%
17	11.804	1648	1652	1659	rBV2	291930	362351	10.73%	1.476%
18	11.886	1663	1666	1673	rVB	28974	43225	1.28%	0.176%
19	12.486	1765	1768	1772	rBV	223455	204597	6.06%	0.833%
20	12.592	1783	1786	1792	rBV2	53847	75771	2.24%	0.309%
21	12.716	1801	1807	1812	rVB	181226	196517	5.82%	0.800%
22	12.863	1827	1832	1835	rBV	2582280	2324671	68.87%	9.468%
23	13.927	2008	2013	2016	rBV2	609458	701110	20.77%	2.856%
24	13.951	2016	2017	2024	rVB	92974	75898	2.25%	0.309%
25	14.086	2037	2040	2043	rBV	37084	37756	1.12%	0.154%
26	14.768	2153	2156	2160	rVB	80788	87365	2.59%	0.356%
27	14.968	2186	2190	2193	rBV	64711	93458	2.77%	0.381%
28	15.268	2238	2241	2246	rBV	39710	44735	1.33%	0.182%
29	15.333	2249	2252	2257	rVB	56566	64225	1.90%	0.262%
30	15.392	2257	2262	2275	rBV	483718	655843	19.43%	2.671%
31	16.880	2512	2515	2521	rVB2	24174	39223	1.16%	0.160%
32	17.333	2588	2592	2598	rVB2	21846	40684	1.21%	0.166%

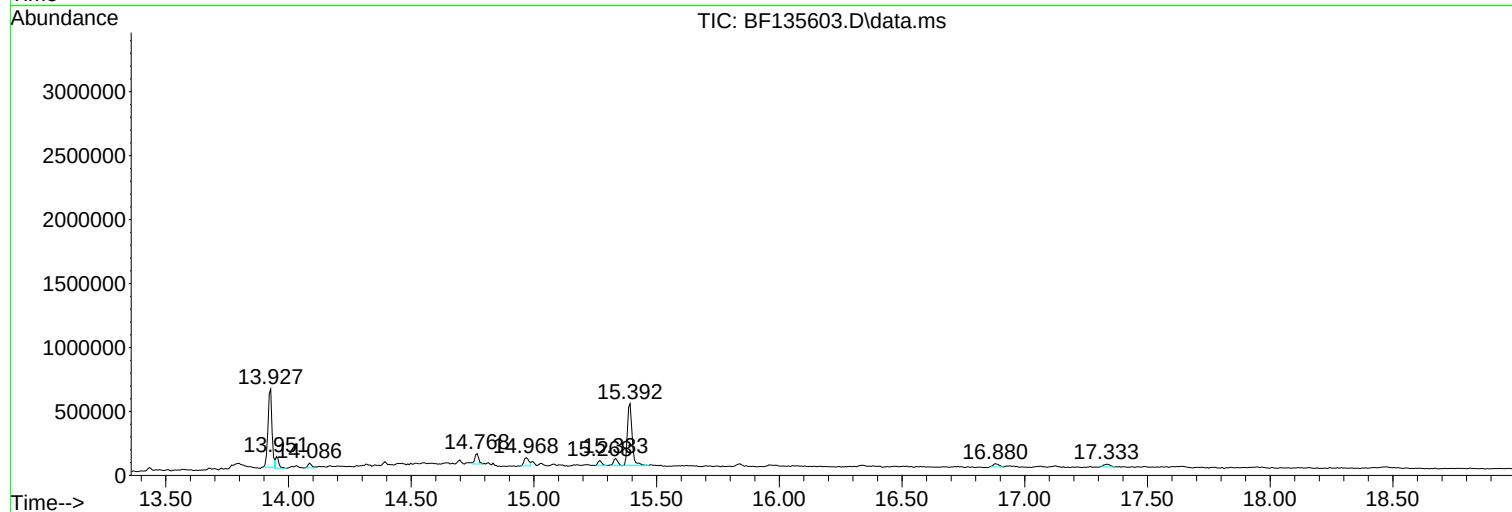
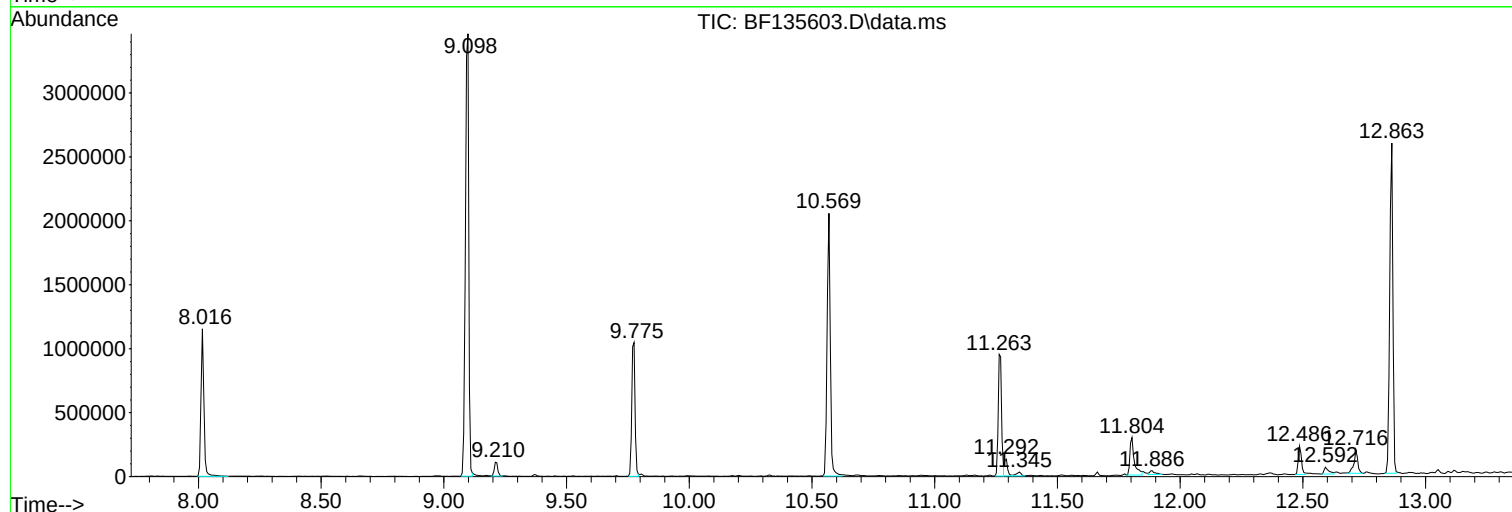
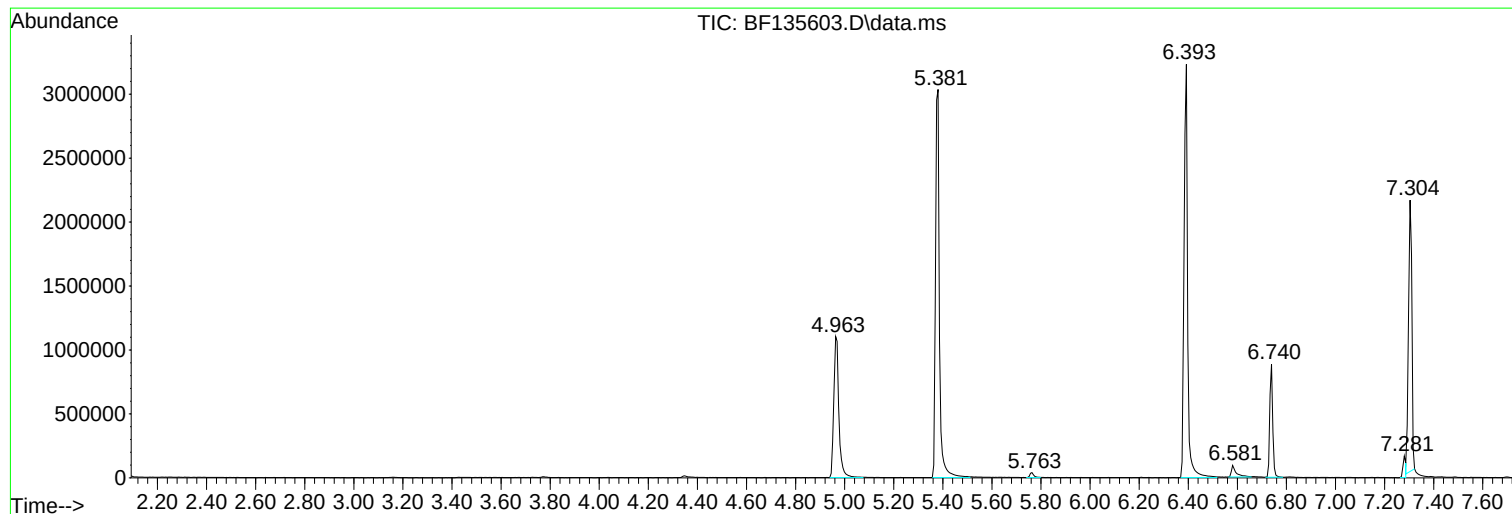
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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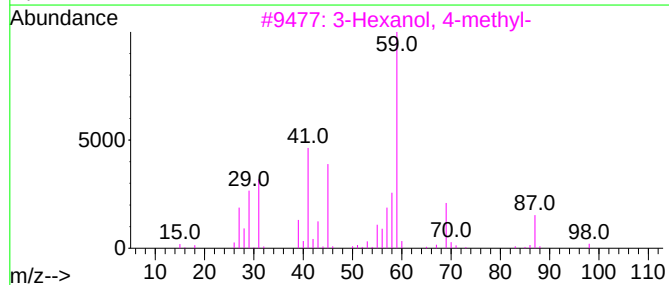
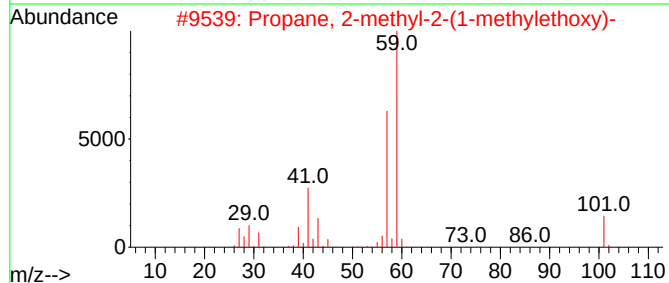
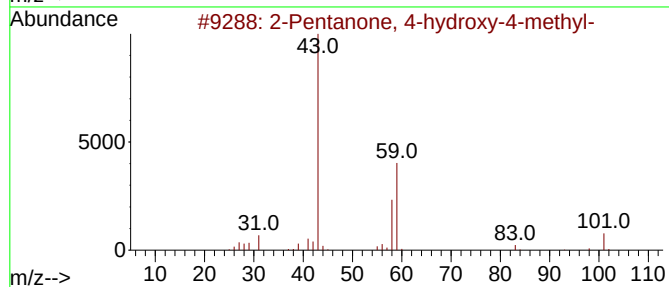
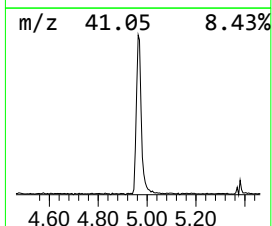
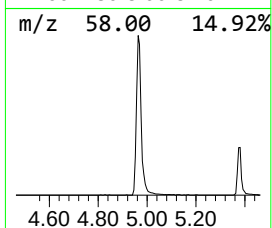
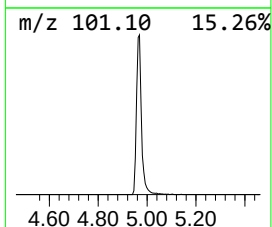
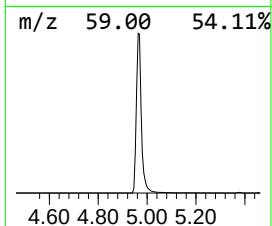
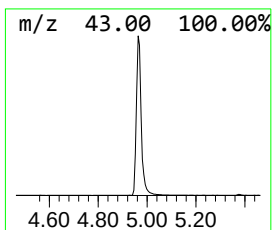
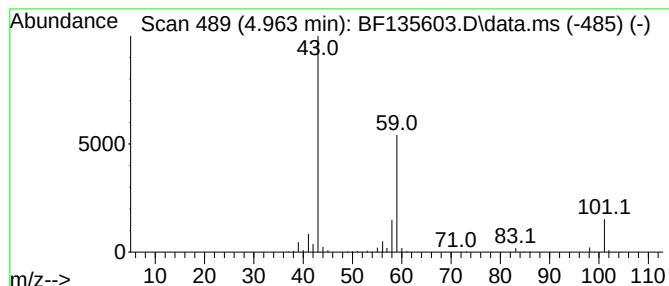
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	42.40 ng	1563190	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



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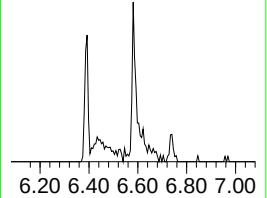
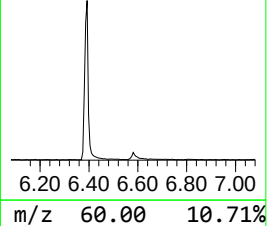
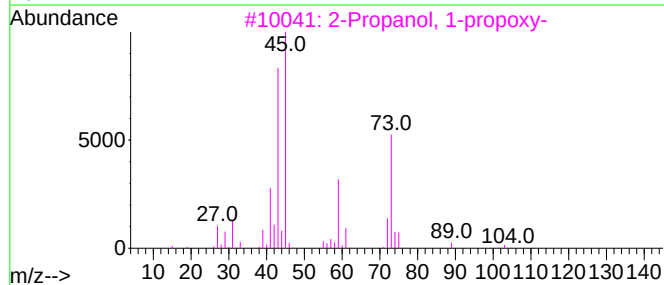
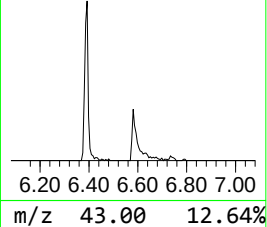
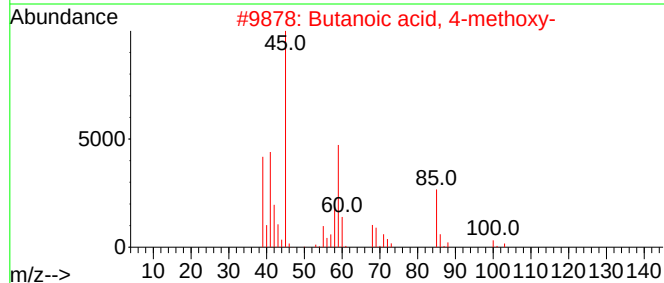
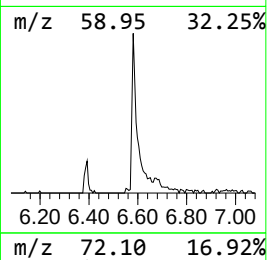
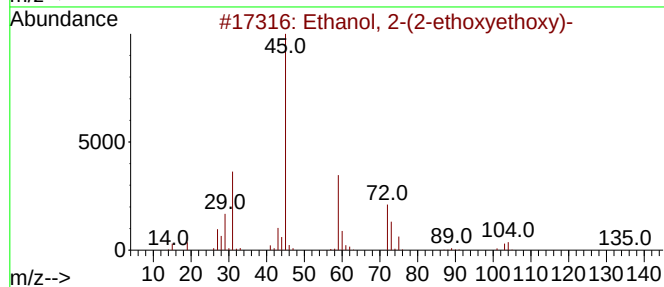
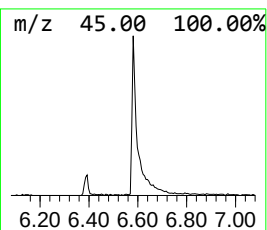
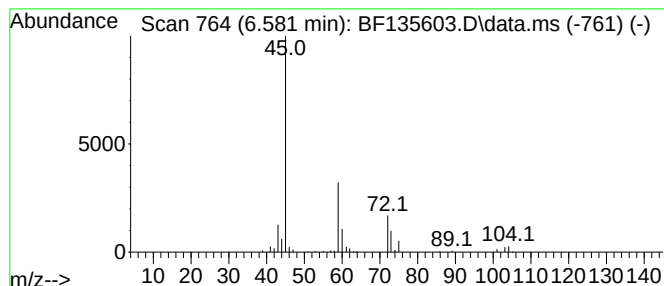
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.581	3.26 ng	120356	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	40
3			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
4			.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	38
5			1-Butaneboronic acid	102	C4H11BO2	004426-47-5	38



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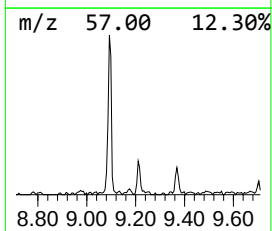
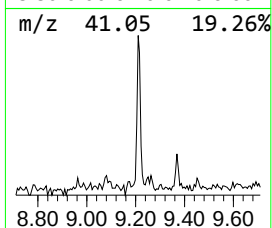
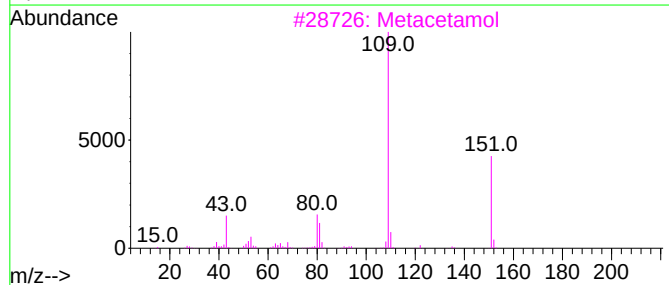
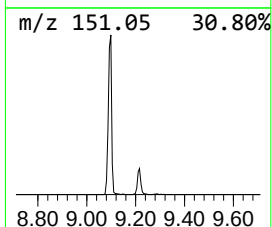
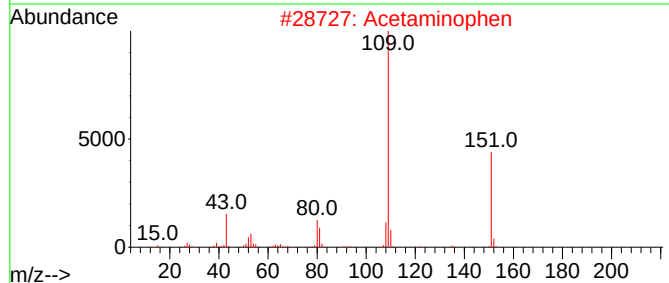
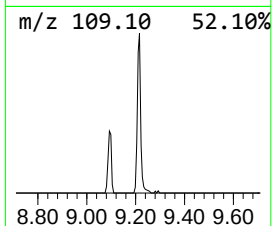
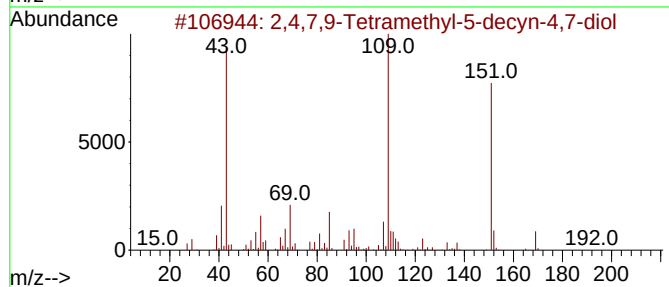
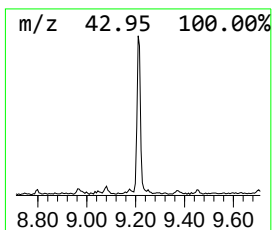
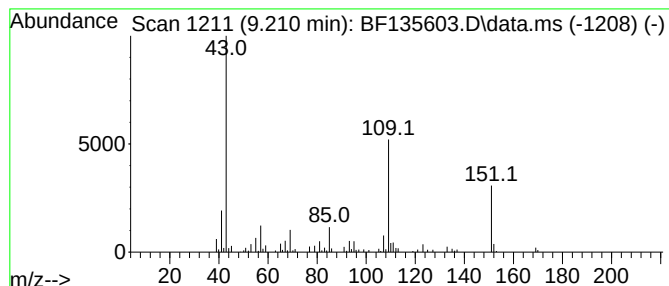
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.210	2.13 ng	103341	Acenaphthene-d10	9.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	86	
2	Acetaminophen	151	C8H9NO2	000103-90-2	49	
3	Metacetamol	151	C8H9NO2	000621-42-1	47	
4	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	43	
5	4-Amino-2-methylpyrimidine	109	C5H7N3	000074-69-1	38	



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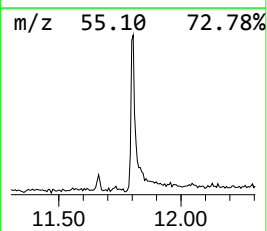
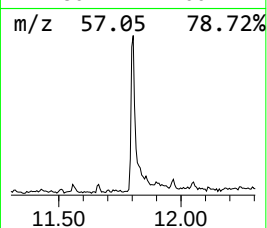
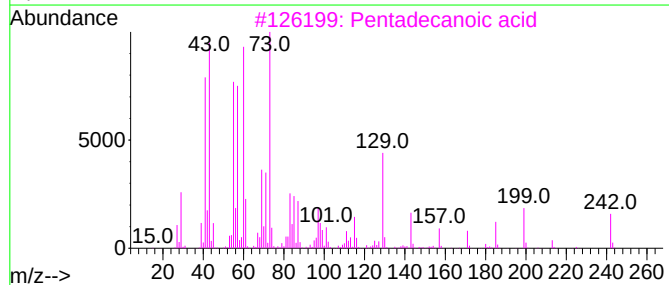
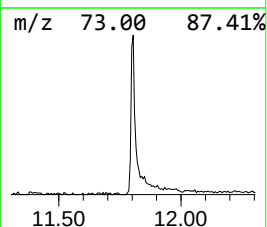
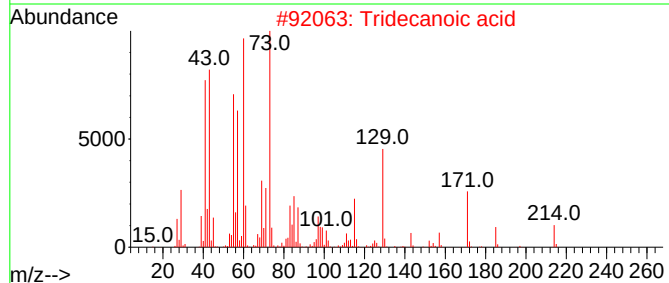
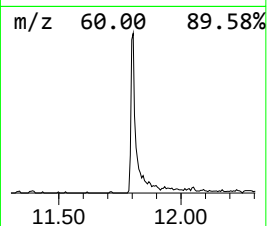
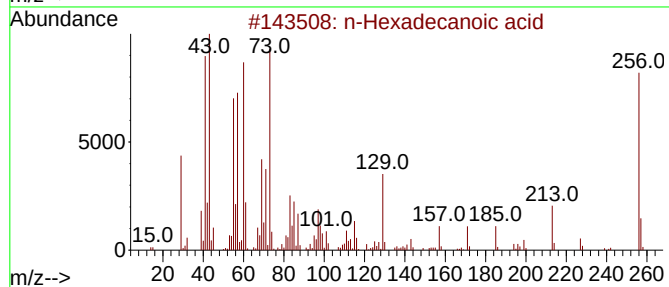
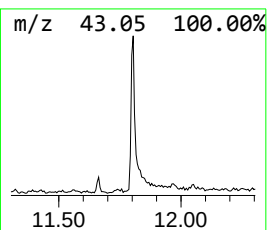
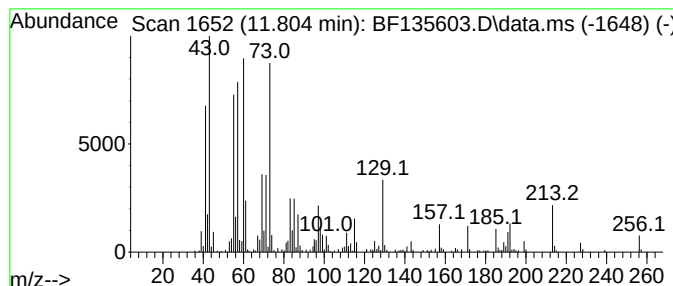
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	8.04 ng	362351	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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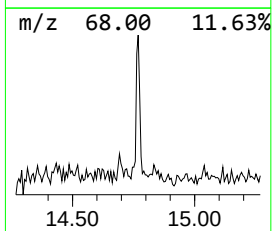
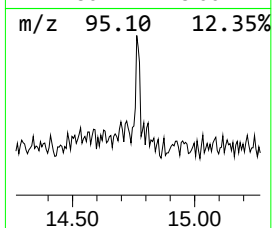
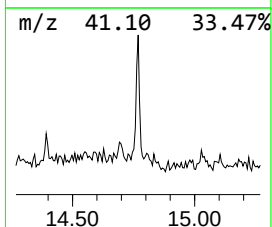
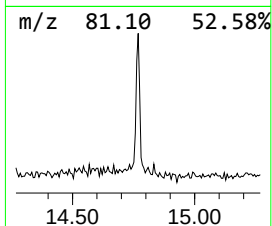
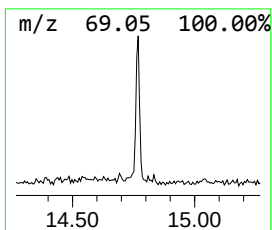
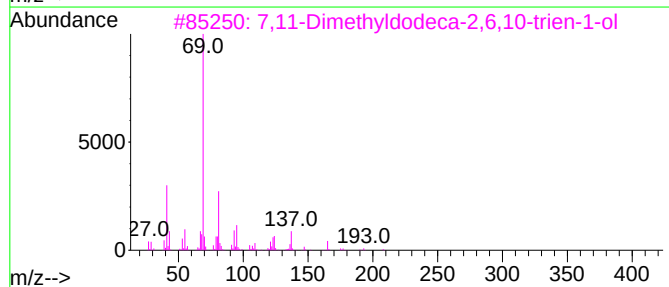
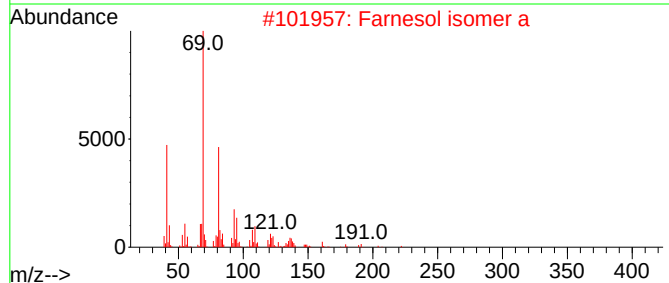
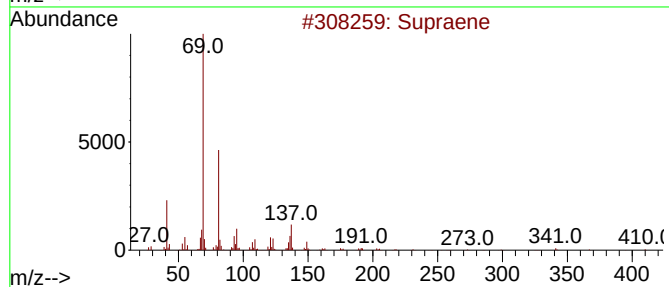
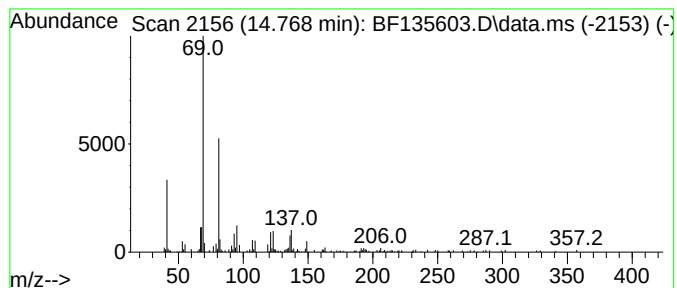
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Peak Number 5 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	2.66 ng	87365	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	86
2			Farnesol isomer a	222	C15H26O	1000108-92-4	80
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	78
5			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.963	42.4	ng	1563190	1	6.740	737335	20.0
Ethanol, 2-(2-e...	6.581	3.3	ng	120356	1	6.740	737335	20.0
2,4,7,9-Tetrame...	9.210	2.1	ng	103341	3	9.775	971056	20.0
n-Hexadecanoic ...	11.804	8.0	ng	362351	4	11.269	901455	20.0
Supraene	14.768	2.7	ng	87365	6	15.392	655843	20.0