

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
 Data File : BF135858.D
 Acq On : 18 Oct 2023 20:54
 Operator : CG\JU
 Sample : 04895-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135858.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	485	488	502	rBV	414914	603904	28.77%	3.887%
2	5.375	556	559	582	rBV	1469266	1789421	85.25%	11.516%
3	6.393	729	732	759	rBV	1922848	2037686	97.08%	13.114%
4	6.616	767	770	777	rBV5	8841	23449	1.12%	0.151%
5	6.740	787	791	802	rVB	541420	498822	23.76%	3.210%
6	7.304	884	887	901	rBV	1226752	1279364	60.95%	8.234%
7	8.016	1005	1008	1025	rVB	703741	656641	31.28%	4.226%
8	9.098	1188	1192	1195	rBV	2258466	2098994	100.00%	13.509%
9	9.210	1208	1211	1228	rVB	292788	311418	14.84%	2.004%
10	9.775	1303	1307	1319	rBV	846174	704955	33.59%	4.537%
11	10.575	1439	1443	1458	rBV	1293841	1315524	62.67%	8.466%
12	11.269	1558	1561	1571	rBV	760866	745287	35.51%	4.797%
13	11.804	1649	1652	1664	rBV2	131560	172027	8.20%	1.107%
14	12.375	1741	1749	1751	rBV2	32148	39839	1.90%	0.256%
15	12.598	1784	1787	1797	rBV3	22703	41448	1.97%	0.267%
16	12.869	1829	1833	1836	rBV	2135156	1864293	88.82%	11.998%
17	13.092	1867	1871	1874	rBV	27513	23685	1.13%	0.152%
18	13.439	1926	1930	1933	rBV	43753	43731	2.08%	0.281%
19	13.769	1982	1986	1992	rBV	45167	42855	2.04%	0.276%
20	13.869	1992	2003	2006	rBV7	20275	60589	2.89%	0.390%
21	13.939	2011	2015	2026	rVV	494466	514266	24.50%	3.310%
22	14.027	2027	2030	2037	rVB	25975	30466	1.45%	0.196%
23	14.086	2037	2040	2044	rBV	36067	35371	1.69%	0.228%
24	14.398	2089	2093	2096	rBV	33859	32344	1.54%	0.208%
25	14.698	2141	2144	2147	rBV	30241	27258	1.30%	0.175%
26	14.768	2153	2156	2161	rVB	64097	65292	3.11%	0.420%
27	15.033	2198	2201	2206	rVB3	23427	24785	1.18%	0.160%
28	15.415	2261	2266	2278	rBV	296915	432007	20.58%	2.780%
29	15.839	2333	2338	2343	rBV7	13259	22308	1.06%	0.144%

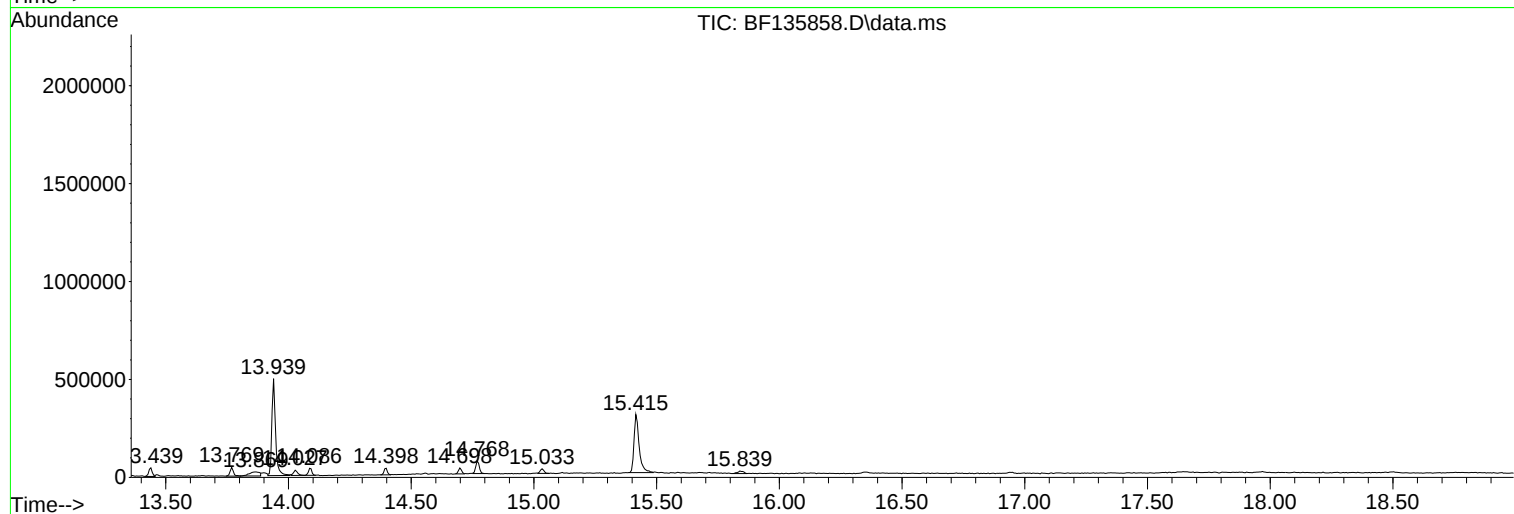
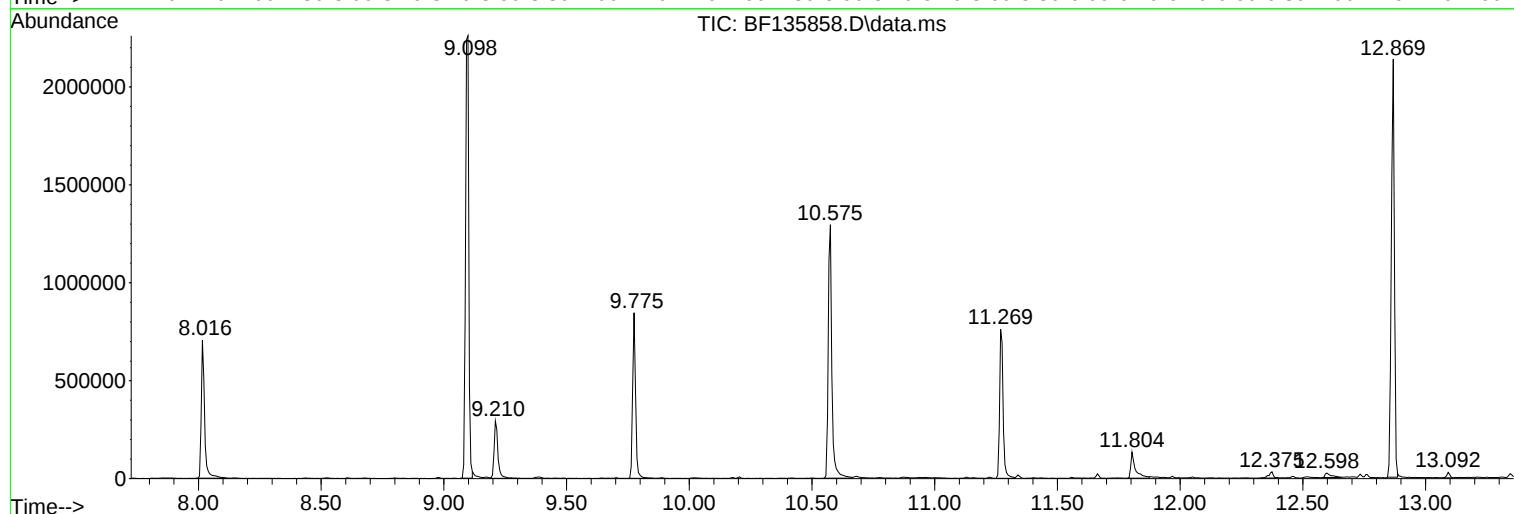
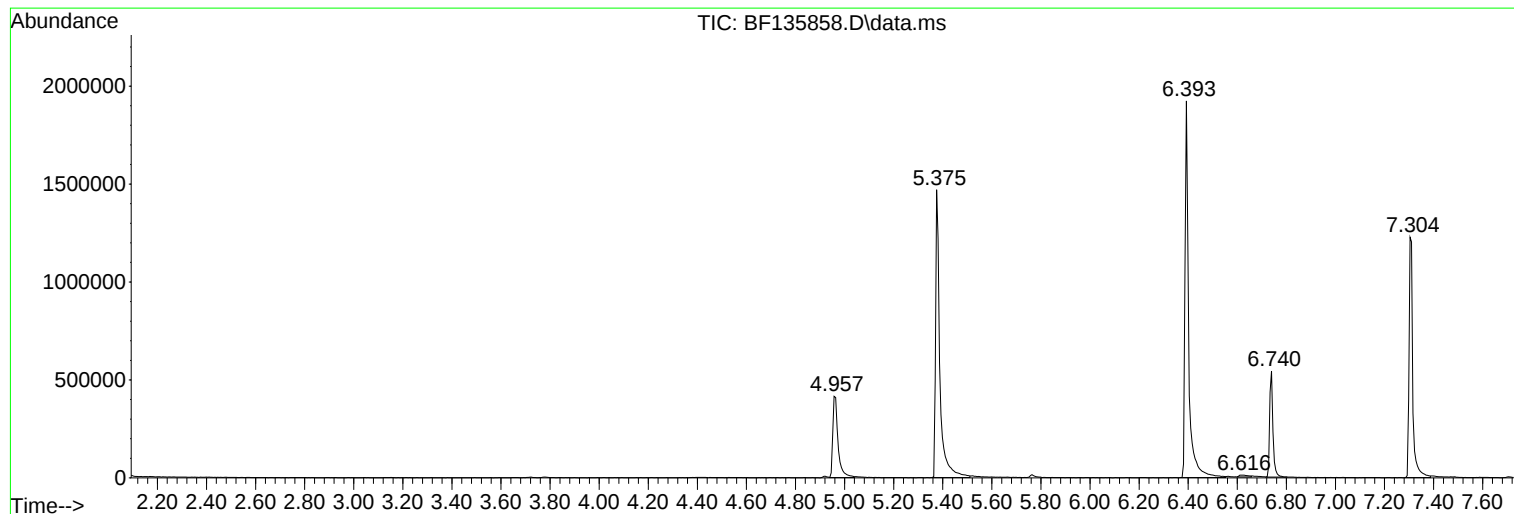
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ALS Vial : 4 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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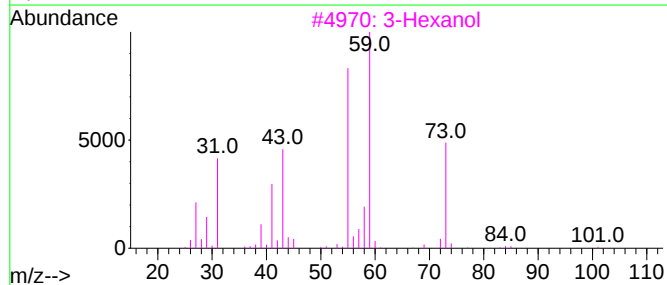
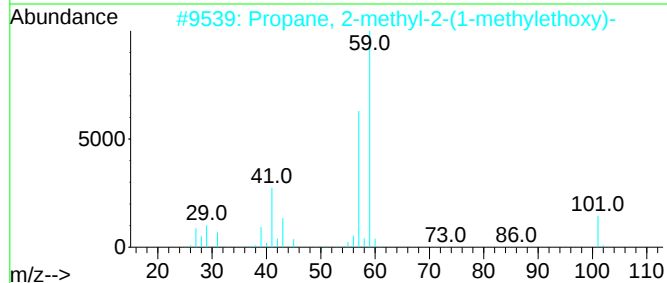
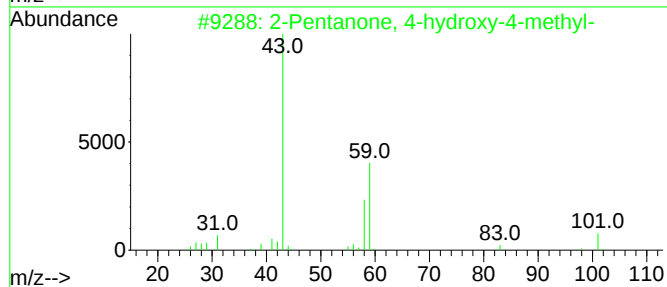
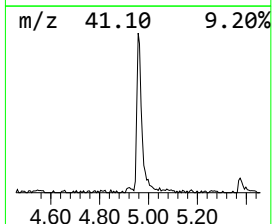
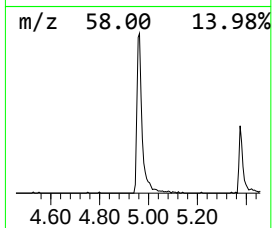
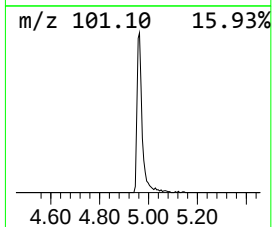
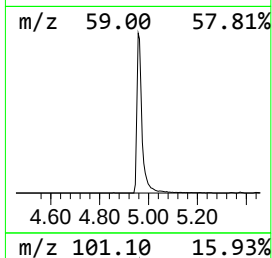
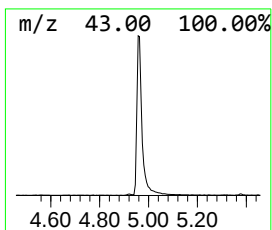
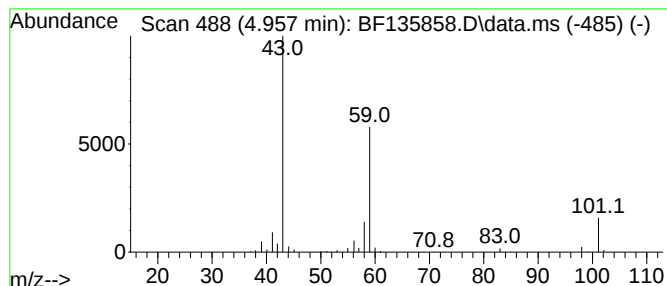
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.957	24.21 ng	603904	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	42
3	3-Hexanol		102	C6H14O	000623-37-0	33
4	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25



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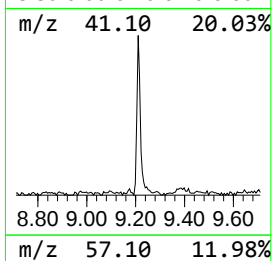
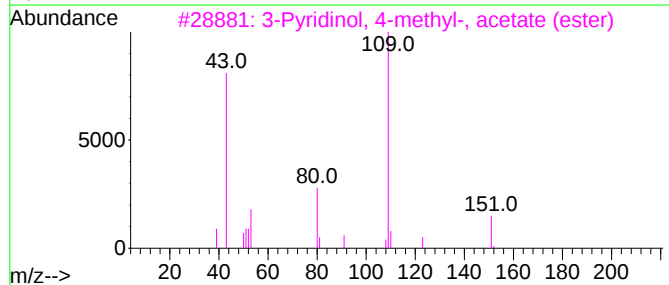
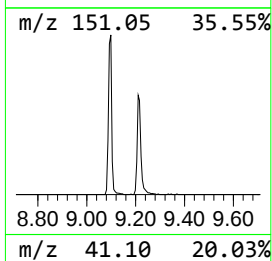
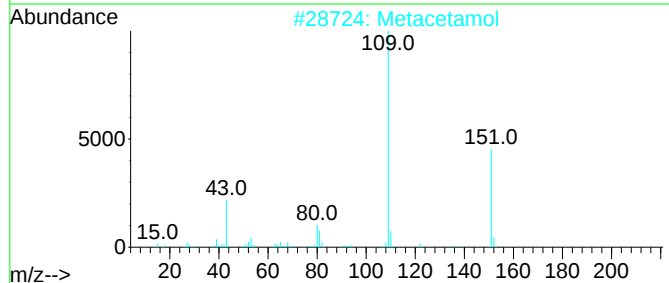
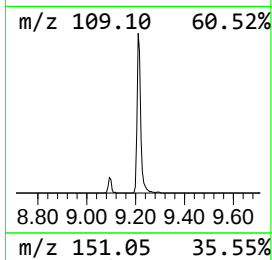
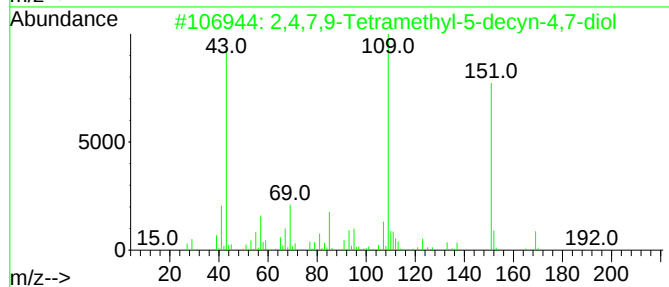
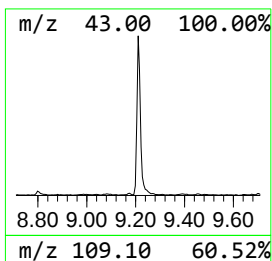
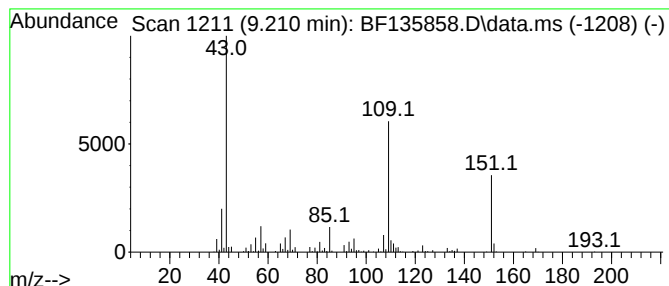
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.210	8.84 ng	311418	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	80	
2	Metacetamol	151	C8H9NO2	000621-42-1	49	
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	47	
4	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	43	
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	42	



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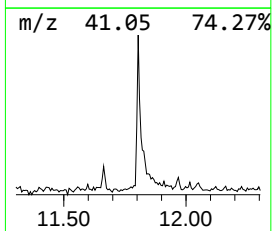
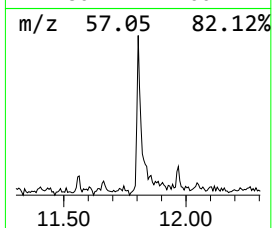
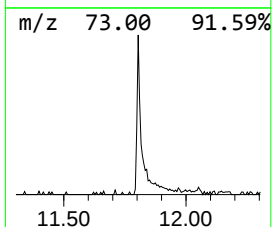
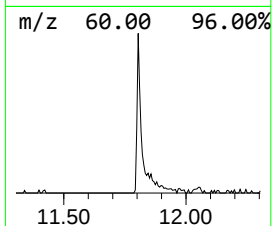
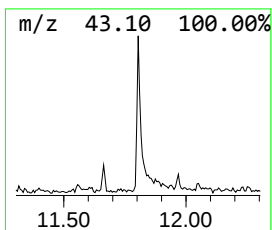
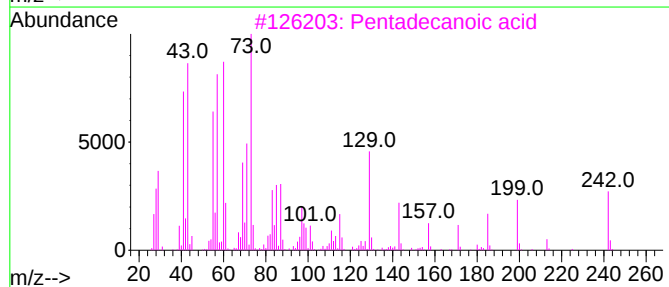
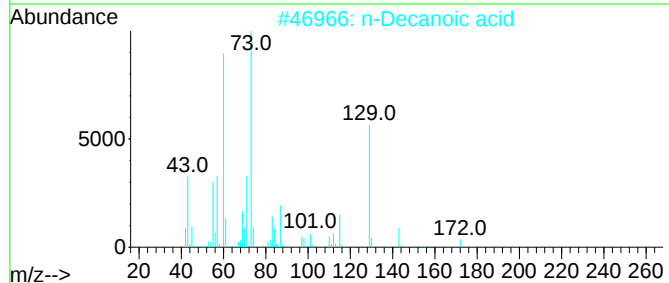
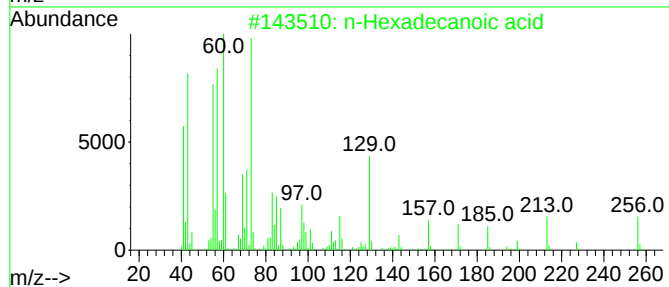
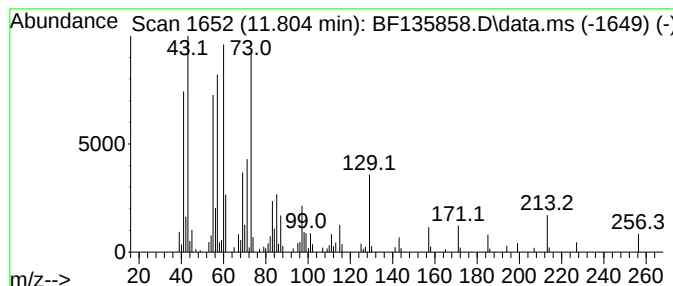
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	4.62 ng	172027	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	70
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Octanoic acid	144	C8H16O2	000124-07-2	45



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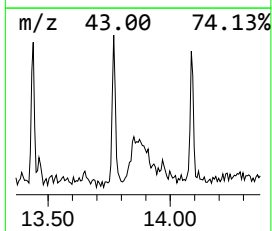
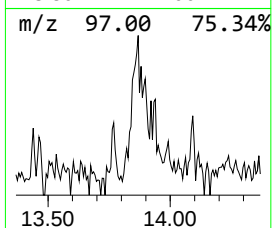
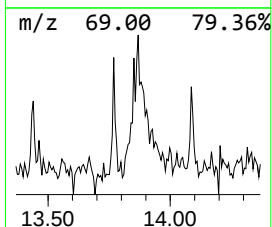
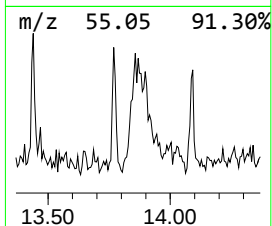
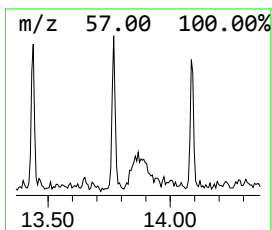
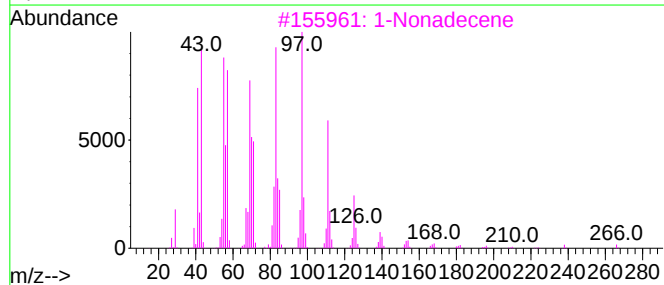
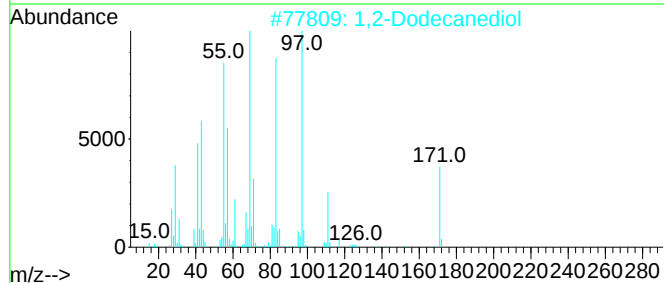
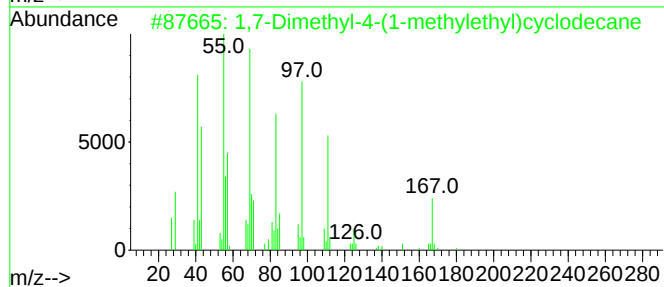
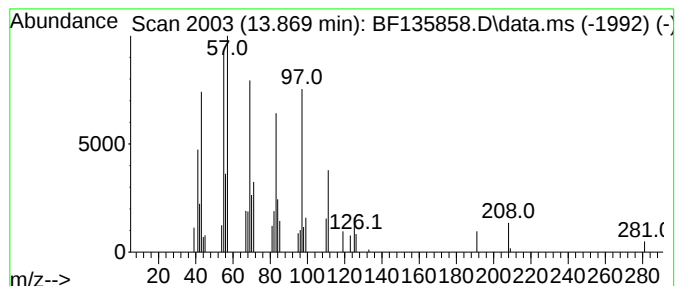
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1,7-Dimethyl-4-(1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.868	2.36 ng	60589	Chrysene-d12	13.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	72
2	1,2-Dodecanediol	202	C12H26O2	001119-87-5	59
3	1-Nonadecene	266	C19H38	018435-45-5	38
4	1-Tricosene	322	C23H46	018835-32-0	38
5	1-Tetracosene	336	C24H48	010192-32-2	38



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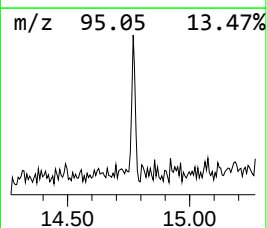
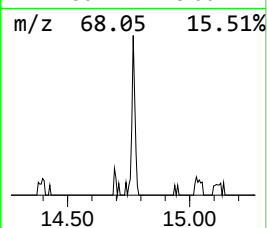
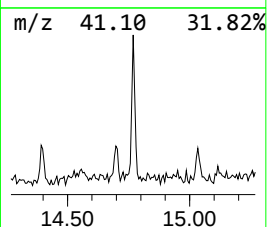
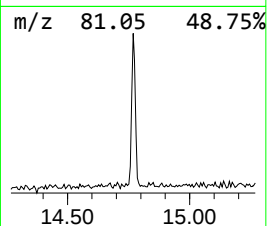
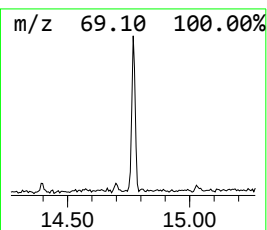
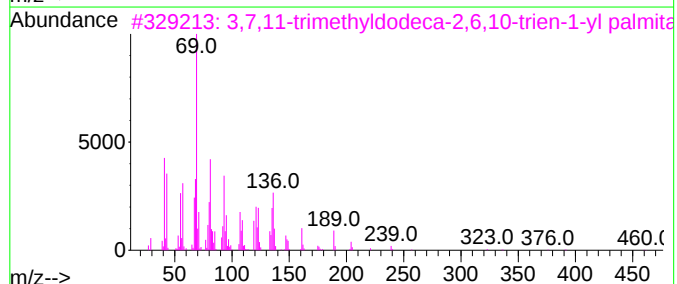
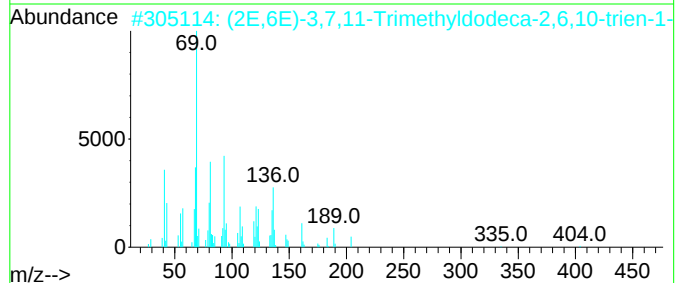
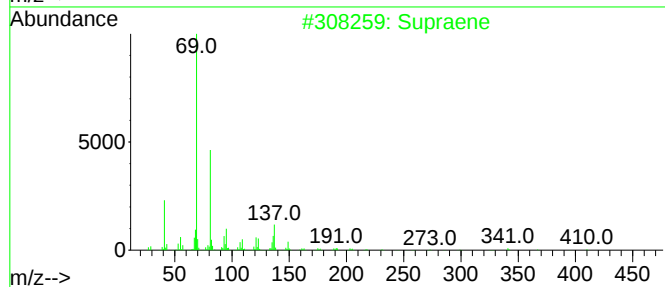
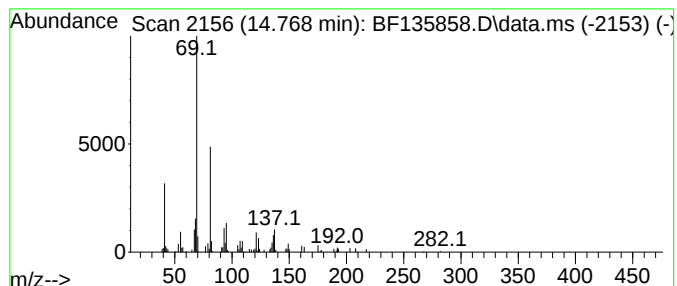
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Peak Number 5 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.769	3.02 ng	65292	Perylene-d12	15.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			(2E,6E)-3,7,11-Trimethyldodeca-2...	404	C27H48O2	078368-58-8	64
3			3,7,11-trimethyldodeca-2,6,10-tr...	460	C31H56O2	157501-12-7	64
4			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	56
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	24.2	ng	603904	1	6.740	498822	20.0
2,4,7,9-Tetrame...	9.210	8.8	ng	311418	3	9.775	704955	20.0
n-Hexadecanoic ...	11.804	4.6	ng	172027	4	11.269	745287	20.0
1,7-Dimethyl-4-...	13.868	2.4	ng	60589	5	13.939	514266	20.0
Supraene	14.769	3.0	ng	65292	6	15.416	432007	20.0