

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
 Data File : BF135205.D
 Acq On : 13 Sep 2023 04:28
 Operator : CG\JU
 Sample : 04343-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-2-23RD-ST

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: BF135205.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	489	493	505	rVB	661893	705338	18.25%	3.499%
2	5.393	558	562	573	rBV	1299679	1185801	30.68%	5.882%
3	6.028	667	670	679	rBV2	35591	64235	1.66%	0.319%
4	6.398	729	733	745	rBV	908978	782971	20.25%	3.884%
5	6.598	764	767	779	rVB	46148	60738	1.57%	0.301%
6	6.763	791	795	798	rBV	821122	688448	17.81%	3.415%
7	7.328	885	891	894	rBV	2156404	2312842	59.83%	11.473%
8	8.039	1008	1012	1016	rBV	1107558	908023	23.49%	4.504%
9	9.122	1191	1196	1199	rBV	4044896	3865648	100.00%	19.176%
10	9.239	1212	1216	1226	rVB	57829	65592	1.70%	0.325%
11	9.551	1265	1269	1273	rBV	50537	44060	1.14%	0.219%
12	9.798	1307	1311	1314	rBV	1236172	1022280	26.45%	5.071%
13	10.592	1441	1446	1449	rBV	1755904	1719933	44.49%	8.532%
14	11.151	1537	1541	1545	rBV2	107313	107001	2.77%	0.531%
15	11.286	1560	1564	1568	rBV	1154625	1064161	27.53%	5.279%
16	11.827	1652	1656	1669	rBV	480147	499729	12.93%	2.479%
17	12.392	1749	1752	1760	rVB2	30409	41672	1.08%	0.207%
18	12.616	1787	1790	1796	rBV	81451	90270	2.34%	0.448%
19	12.892	1831	1837	1840	rBV	3228531	3316758	85.80%	16.453%
20	13.821	1991	1995	2005	rBV	120286	217100	5.62%	1.077%
21	13.945	2011	2016	2020	rBV	590886	599234	15.50%	2.973%
22	14.580	2121	2124	2130	rBV	131084	114858	2.97%	0.570%
23	15.404	2259	2264	2270	rBV	507952	624111	16.15%	3.096%
24	16.015	2362	2368	2377	rVB	20269	58346	1.51%	0.289%

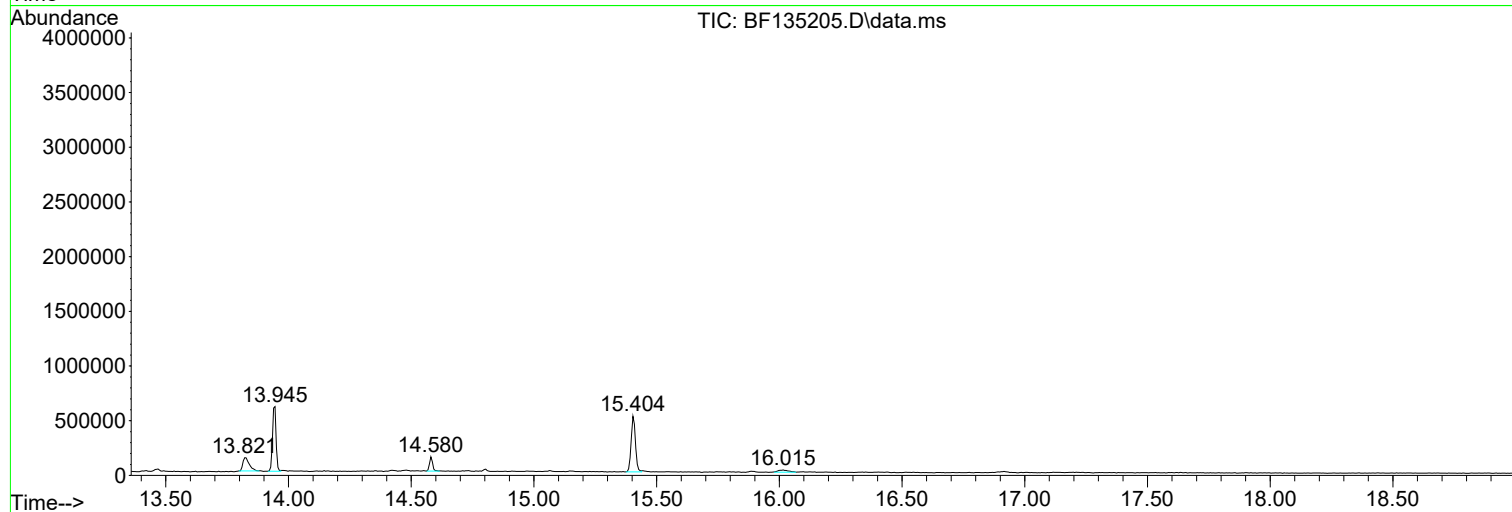
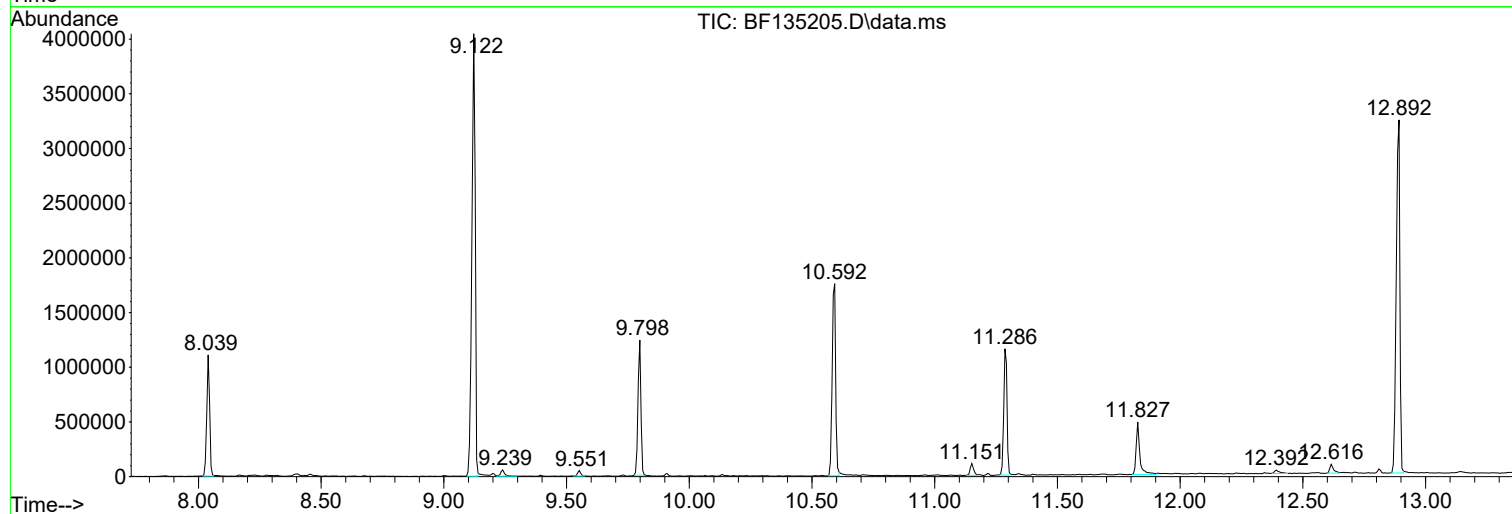
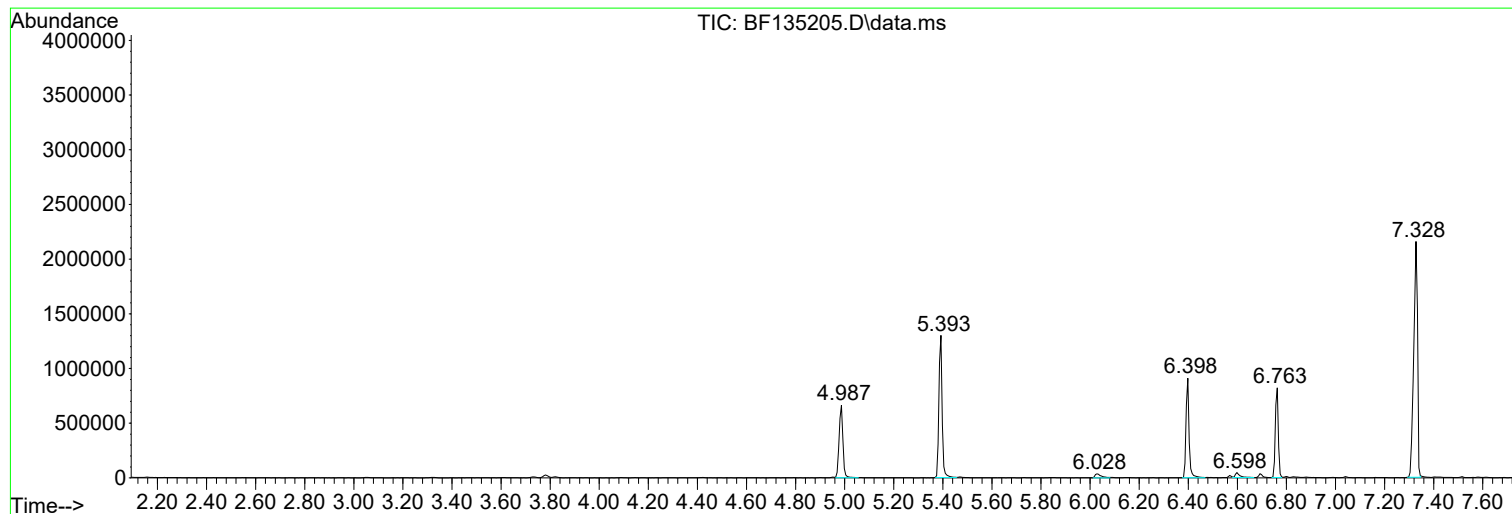
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ALS Vial : 20 Sample Multiplier: 1

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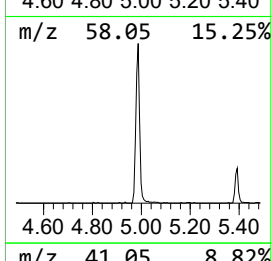
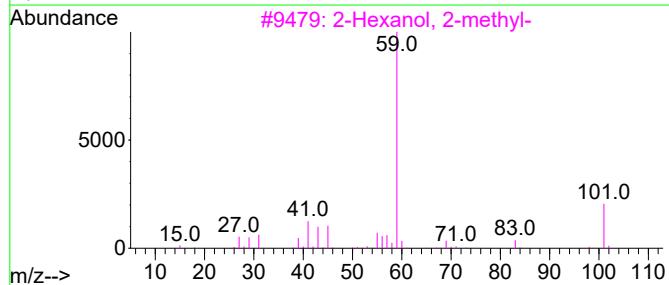
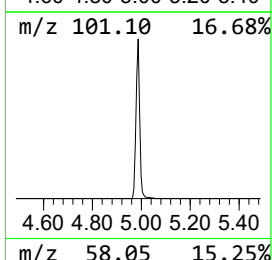
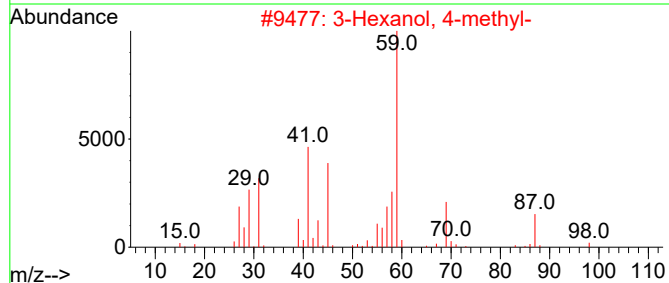
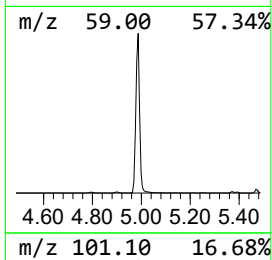
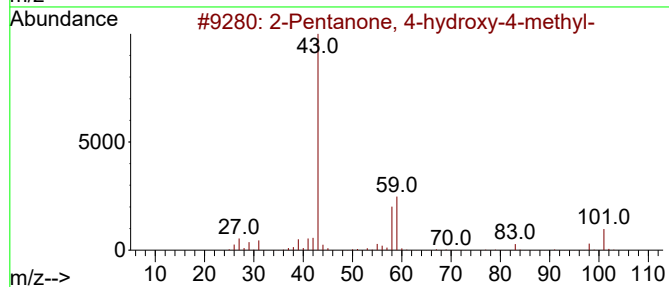
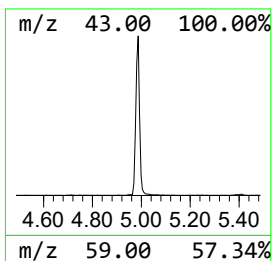
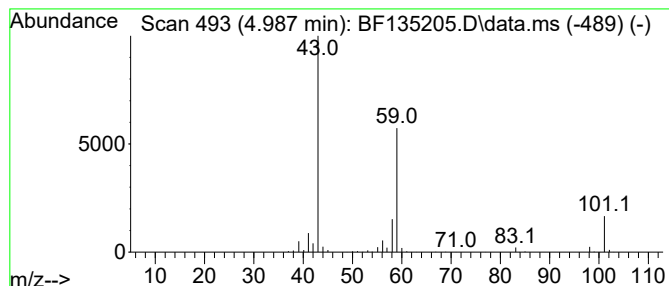
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	20.49 ng	705338	1,4-Dichlorobenzene-d4	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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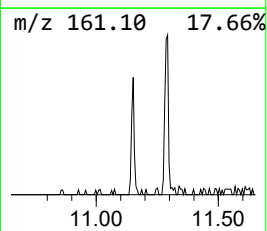
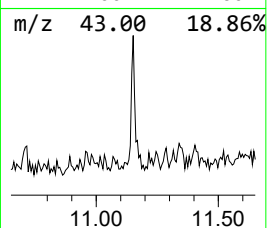
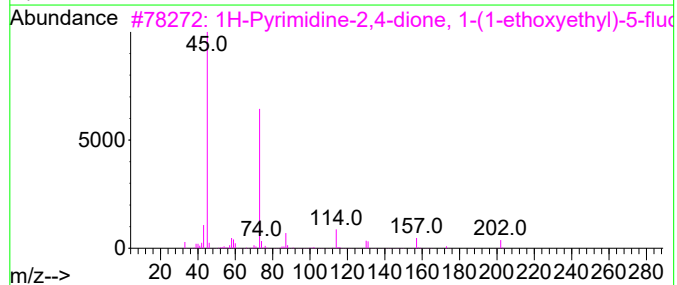
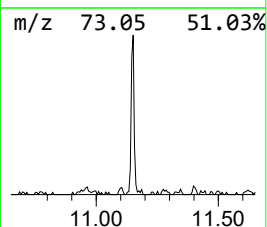
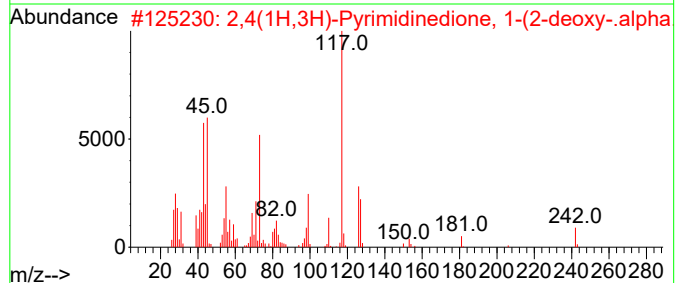
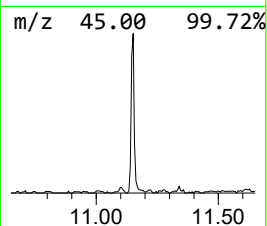
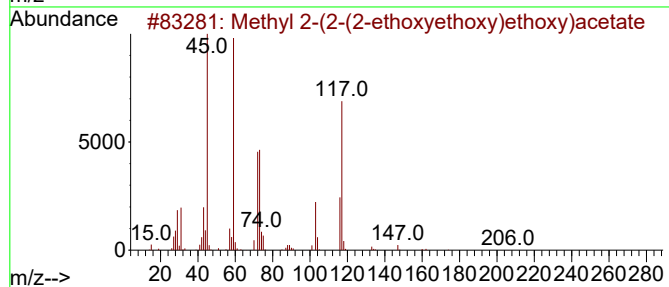
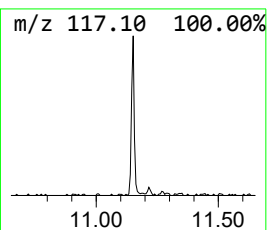
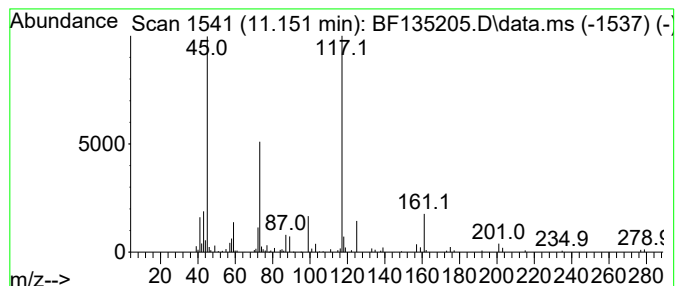
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Peak Number 2 unknown11.151 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.151	2.01 ng	107001	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 2-(2-(2-ethoxyethoxy)etho...	206	C9H18O5	1000366-78-1	38
2			2,4(1H,3H)-Pyrimidinedione, 1-(2...	242	C10H14N2O5	004449-43-8	33
3			1H-Pyrimidine-2,4-dione, 1-(1-et...	202	C8H11FN2O3	1010310-13-3	27
4			Dimethyl 3,6,9,12,15,18,21,24-oc...	470	C20H38O12	1000366-80-8	25
5			Methyl 2,2-dimethyl-3,6,9,12,15,...	426	C18H38O9Si	1000366-82-3	23



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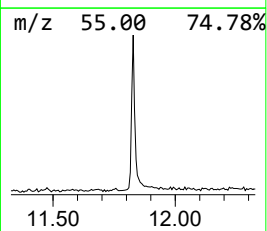
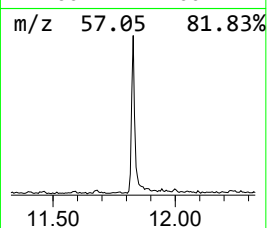
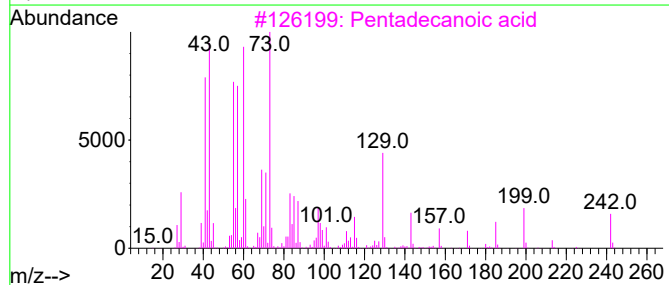
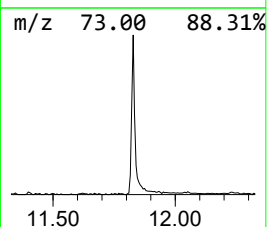
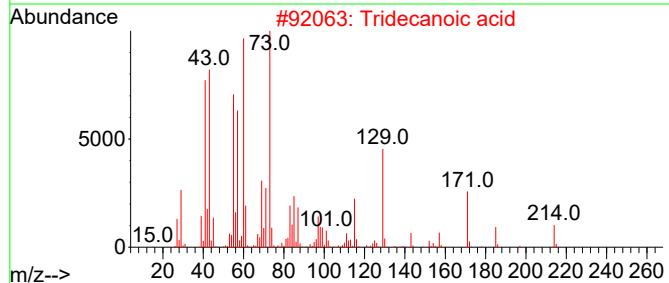
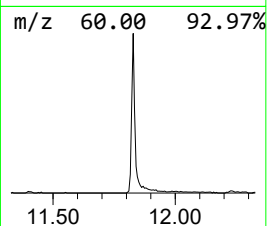
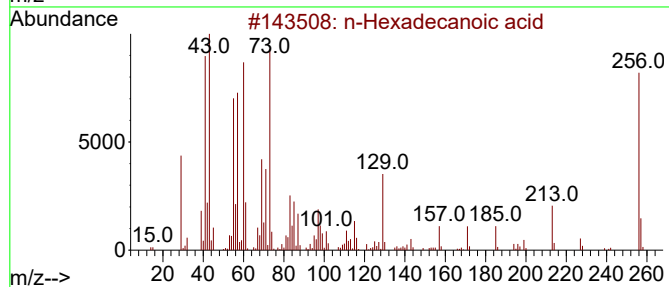
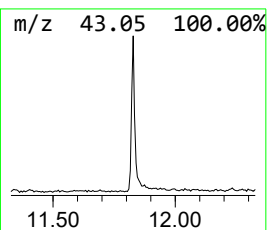
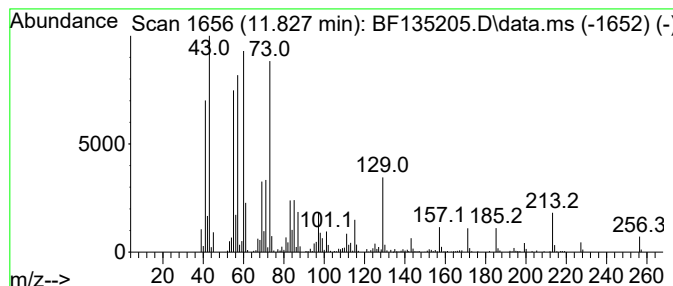
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.828	9.39 ng	499729	Phenanthrene-d10	11.286

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Dodecanoic acid	200	C12H24O2	000143-07-7	74
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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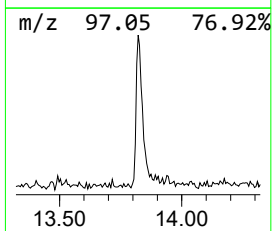
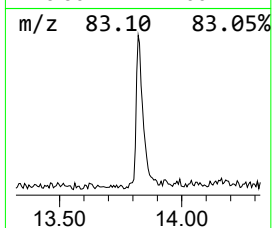
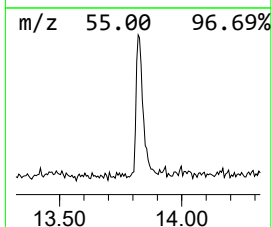
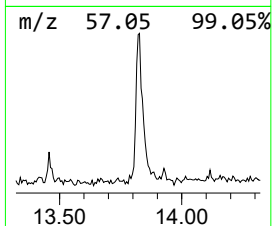
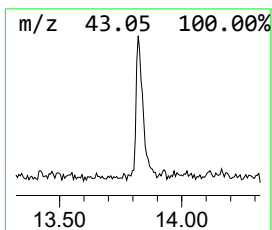
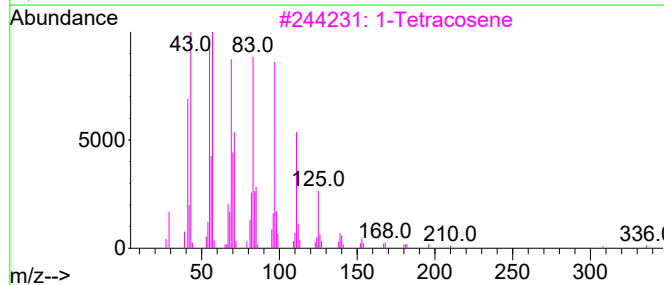
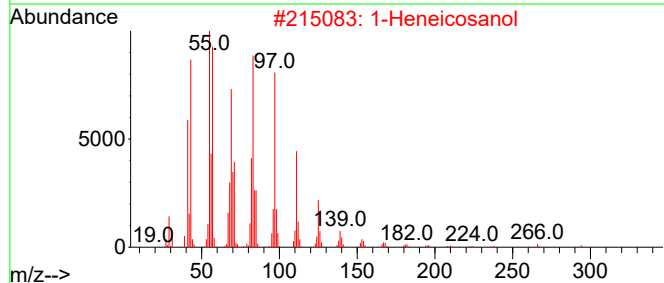
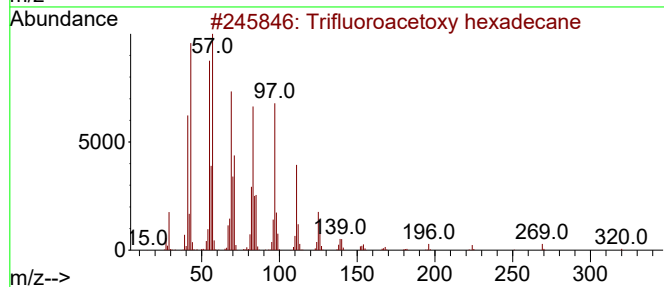
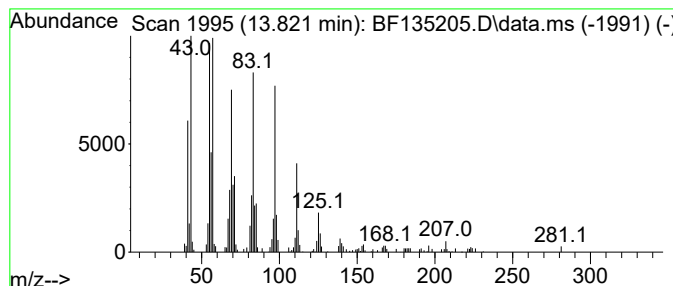
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	7.25 ng	217100	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2			1-Heneicosanol	312	C21H44O	015594-90-8	91
3			1-Tetracosene	336	C24H48	010192-32-2	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91



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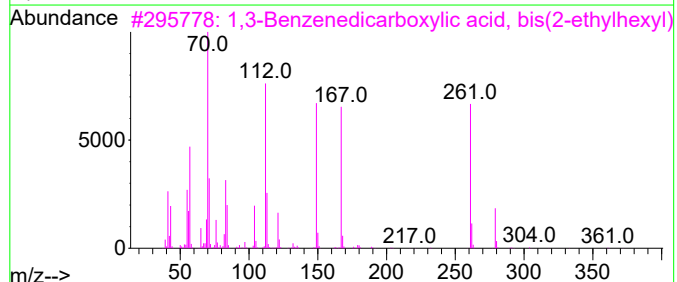
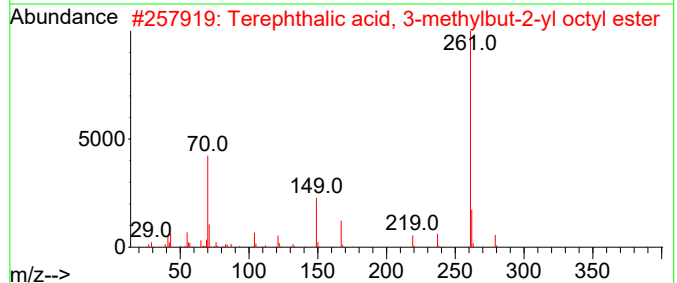
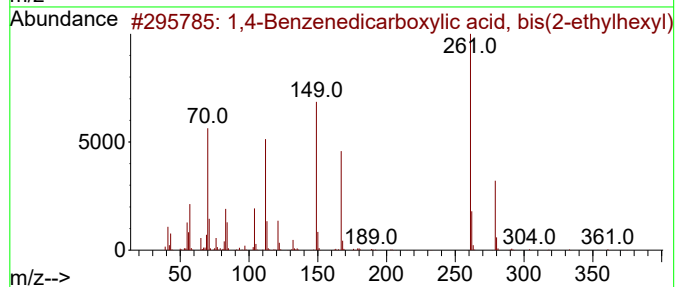
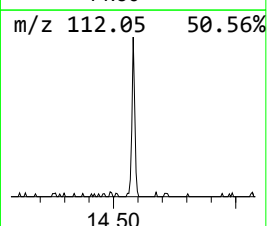
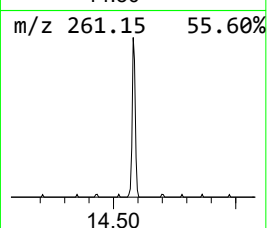
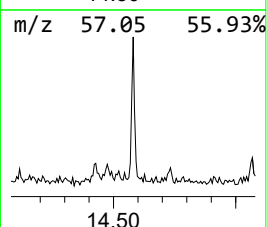
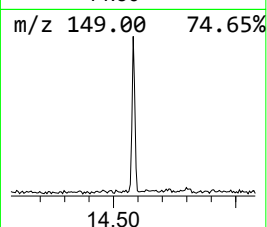
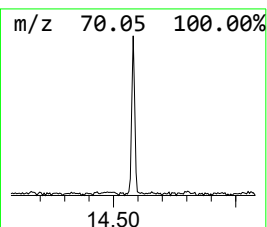
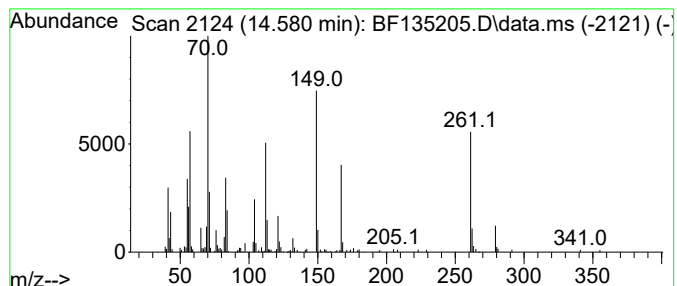
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Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	3.83 ng	114858	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	83
2			Terephthalic acid, 3-methylbut-2...	348	C21H3204	1000356-27-6	72
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	62
4			Terephthalic acid, 4-octyl octyl...	390	C24H3804	1000323-73-7	49
5			Bis(2-ethylhexyl) phthalate	390	C24H3804	000117-81-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	20.5	ng	705338	1	6.763	688448	20.0
unknown11.151	11.151	2.0	ng	107001	4	11.286	1064160	20.0
n-Hexadecanoic ...	11.828	9.4	ng	499729	4	11.286	1064160	20.0
Trifluoroacetox...	13.821	7.3	ng	217100	5	13.945	599234	20.0
1,4-Benzenedica...	14.580	3.8	ng	114858	5	13.945	599234	20.0