LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052623\
Data File : BF133506.D
Acq On : 26 May 2023 18:58
Operator : CG\JU
Sample : 02955-15
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TWP05

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-BF052523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	17	21	30	rVB	63053	80711	2.04%	0.366%
2	4.416	392	396	403	rVB	100418	111149	2.80%	0.503%
3	5.040	497	502	506	rBV	860640	937579	23.65%	4.246%
4	5.440	566	570	573	rBV	1255206	1063662	26.83%	4.817%
5	5.846	636	639	643	rVB	91851	77721	1.96%	0.352%
6	6.445	737	741	750	rBV	819661	676812	17.07%	3.065%
7	6.834	804	807	811	rBV	1061187	842321	21.25%	3.815%
8	7.404	896	904	906	rBV	2281610	2325556	58.67%	10.532%
9	8.122	1022	1026	1029	rBV	1254370	1102976	27.83%	4.995%
10	9.198	1204	1209	1212	rBV	4487849	3920743	98.91%	17.756%
11	9.875	1320	1324	1327	rBV	1415537	1142792	28.83%	5.175%
12	10.586	1442	1445	1449	rBV	654078	514118	12.97%	2.328%
13	10.663	1453	1458	1461	rBV	1690748	1598000	40.31%	7.237%
14	10.898	1495	1498	1502	rVB	86872	72744	1.84%	0.329%
15	11.363	1573	1577	1580	rBV	1277242	1190357	30.03%	5.391%
16	11.892	1663	1667	1671	rBV	215979	214728	5.42%	0.972%
17	12.680	1798	1801	1814	rBV	70876	98584	2.49%	0.446%
18	12.957	1842	1848	1851	rBV	3928931	3963895	100.00%	17.951%
19	13.880	1999	2005	2021	rBV3	82618	218269	5.51%	0.988%
20	13.998	2021	2025	2029	rBV	1041425	1013128	25.56%	4.588%
21	14.639	2130	2134	2138	rVB	144411	126109	3.18%	0.571%
22	15.457	2268	2273	2279	rBV	653424	789679	19.92%	3.576%

Sum of corrected areas: 22081633

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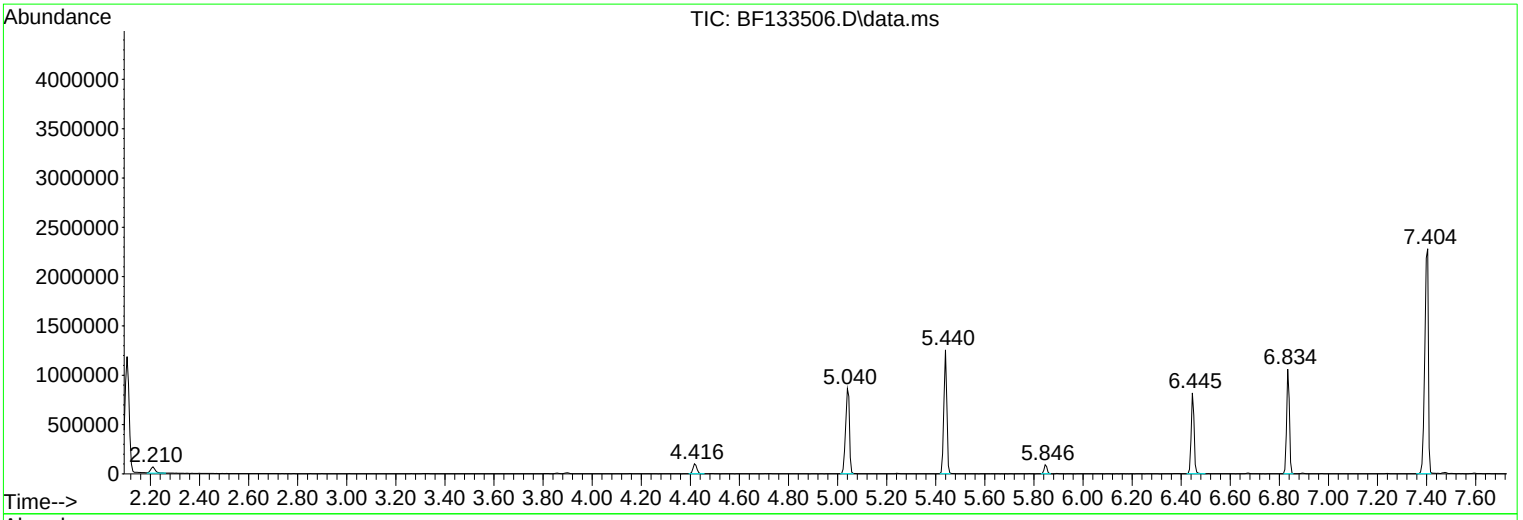
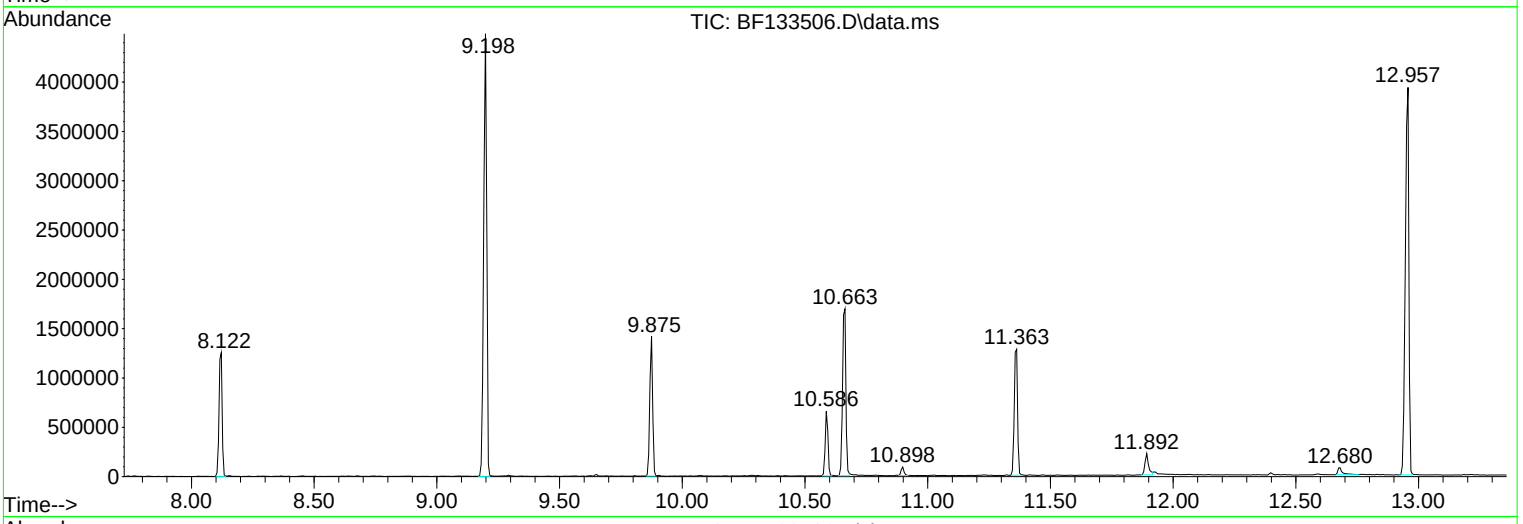
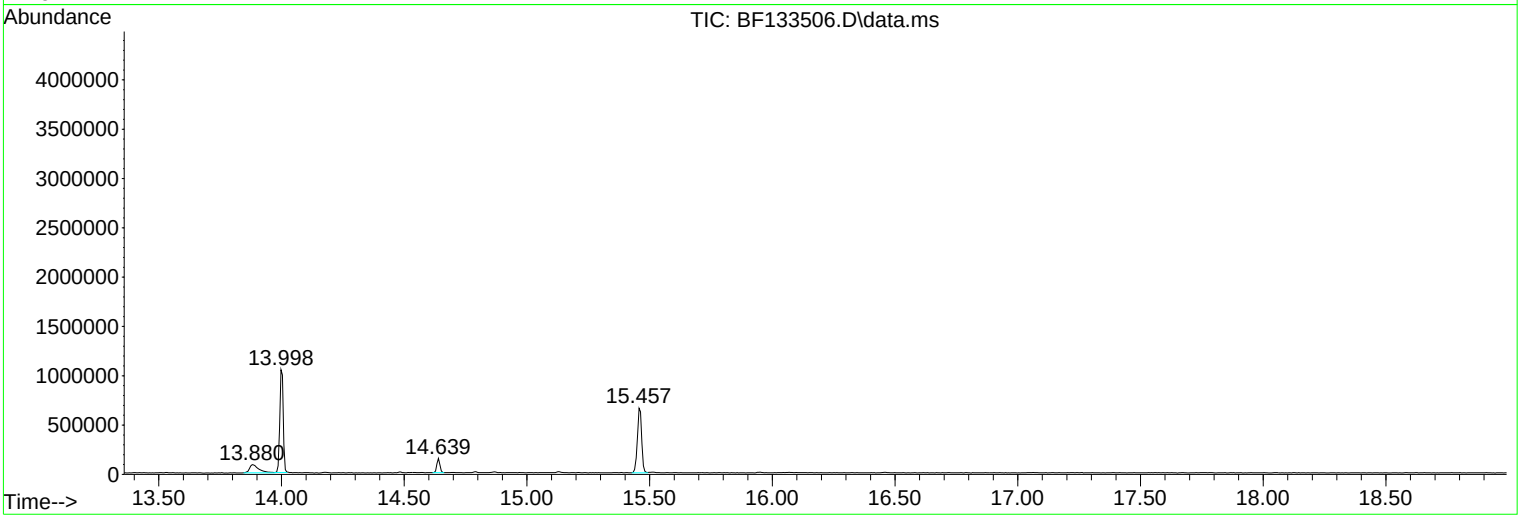
ClientSampleId :
TWP05

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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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TIC Library : C:\Database\NIST20.L
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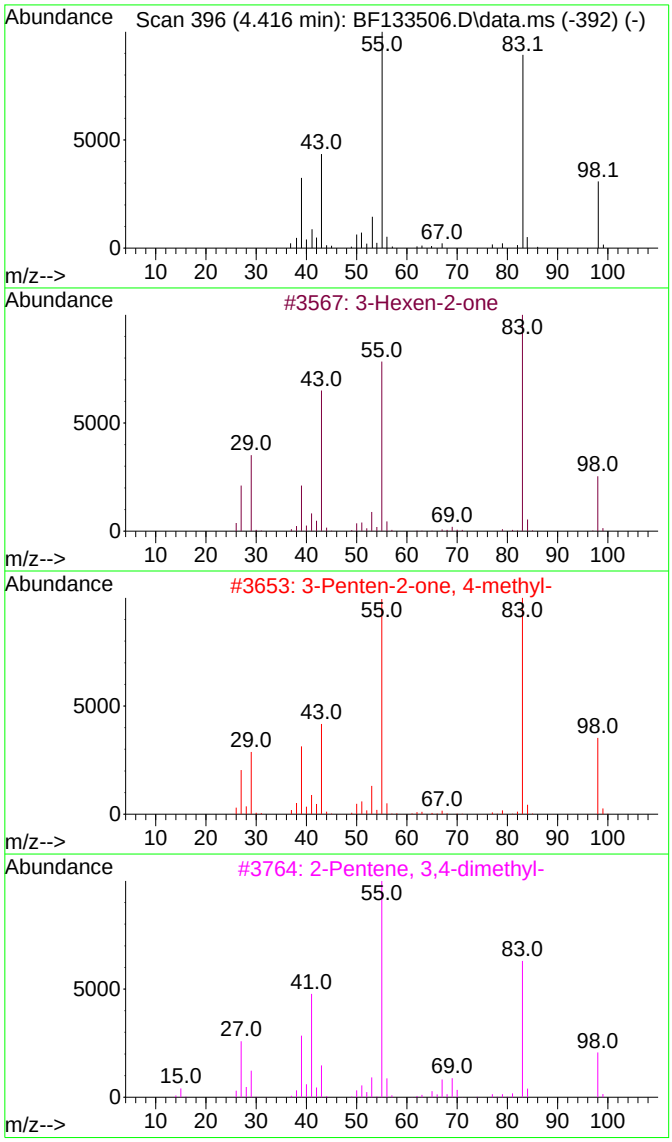
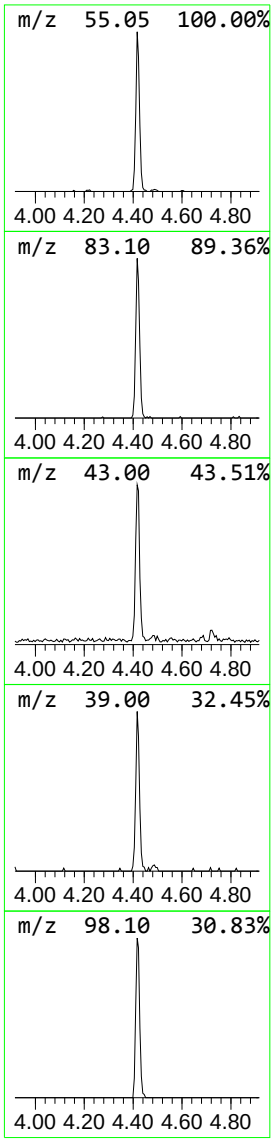
****

Peak Number 1 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	2.64 ng	111149	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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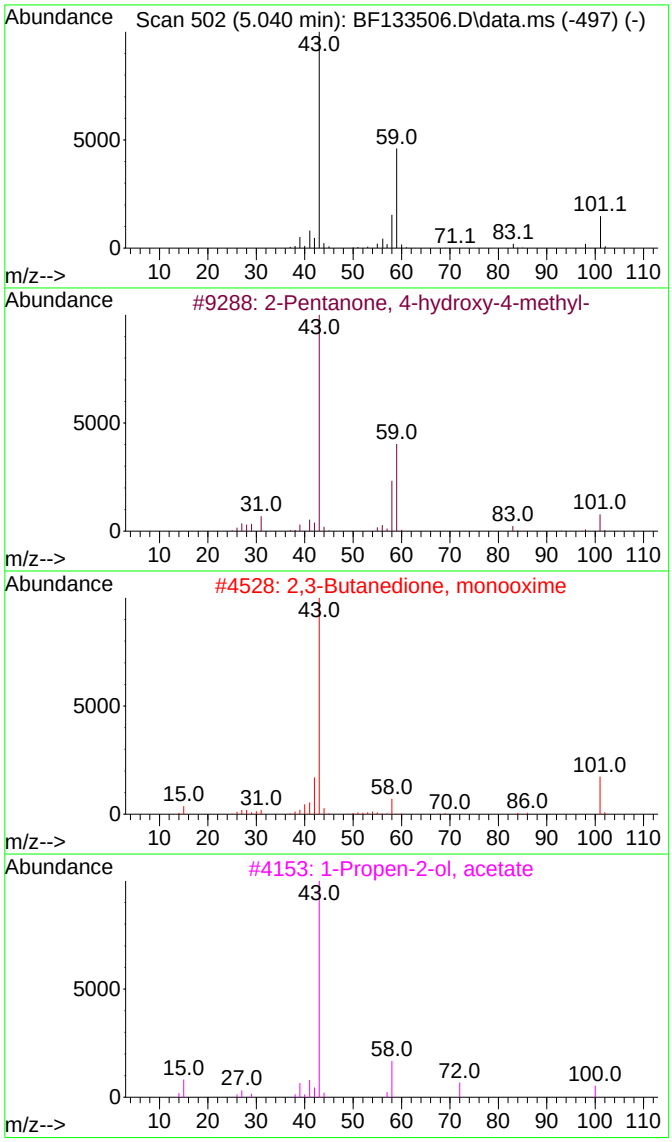
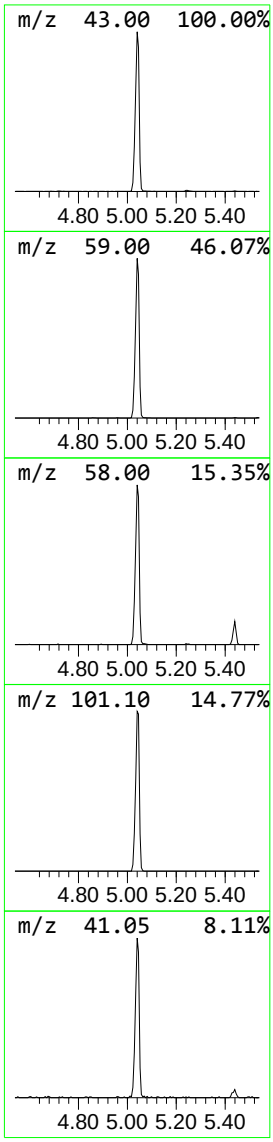
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	22.26 ng	937579	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	Allyl acetate	100	C5H8O2	000591-87-7	9





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Sample : 02955-15
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Instrument :
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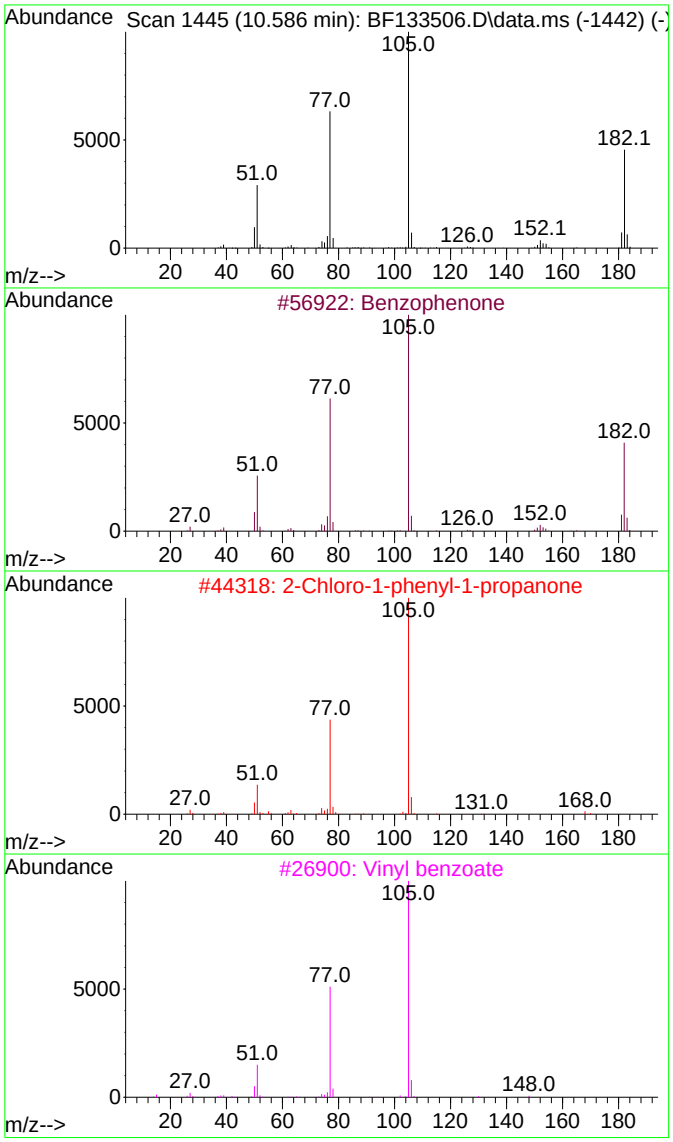
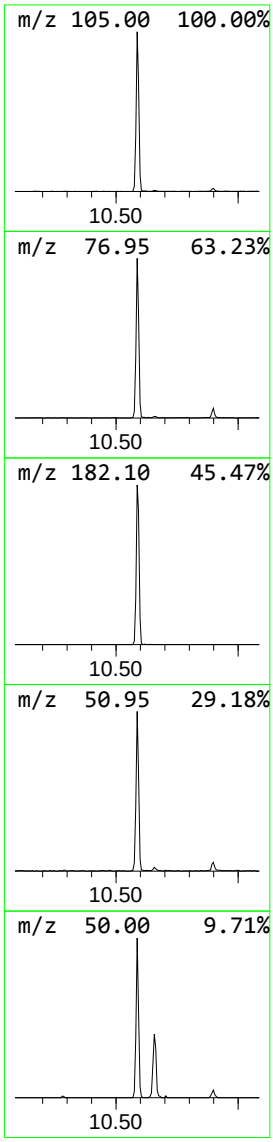
Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	9.00 ng	514118	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	50
3	Vinyl benzoate	148	C9H8O2	000769-78-8	50
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	50





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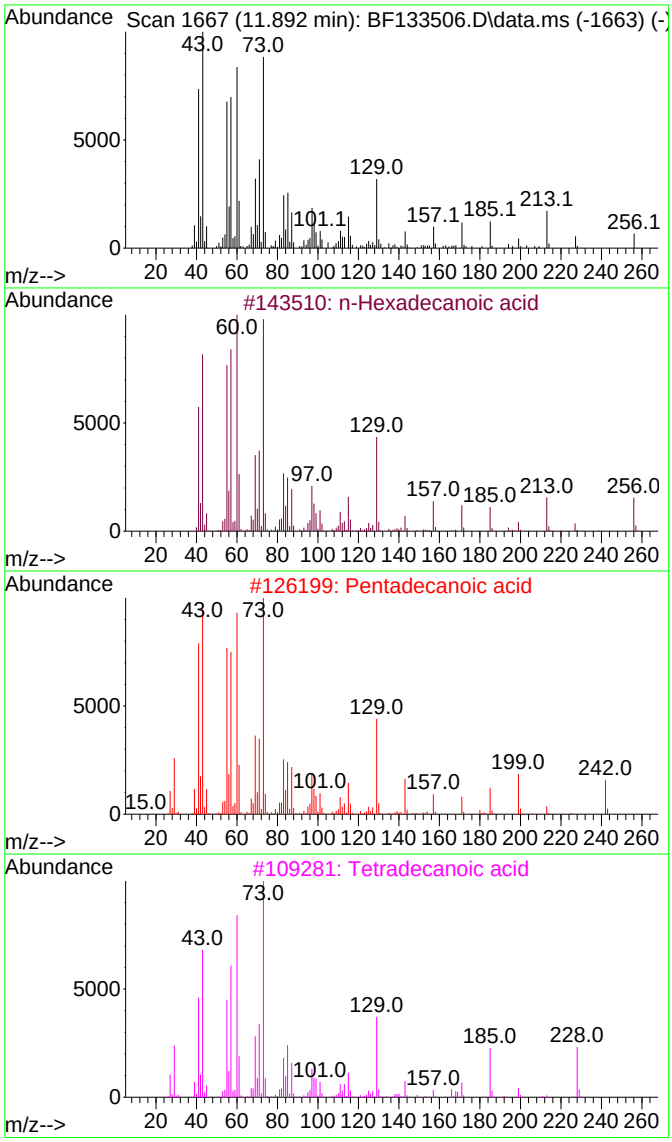
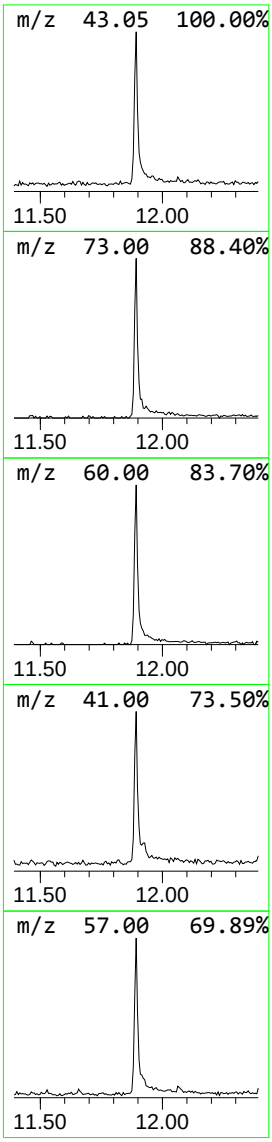
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	3.61 ng	214728	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





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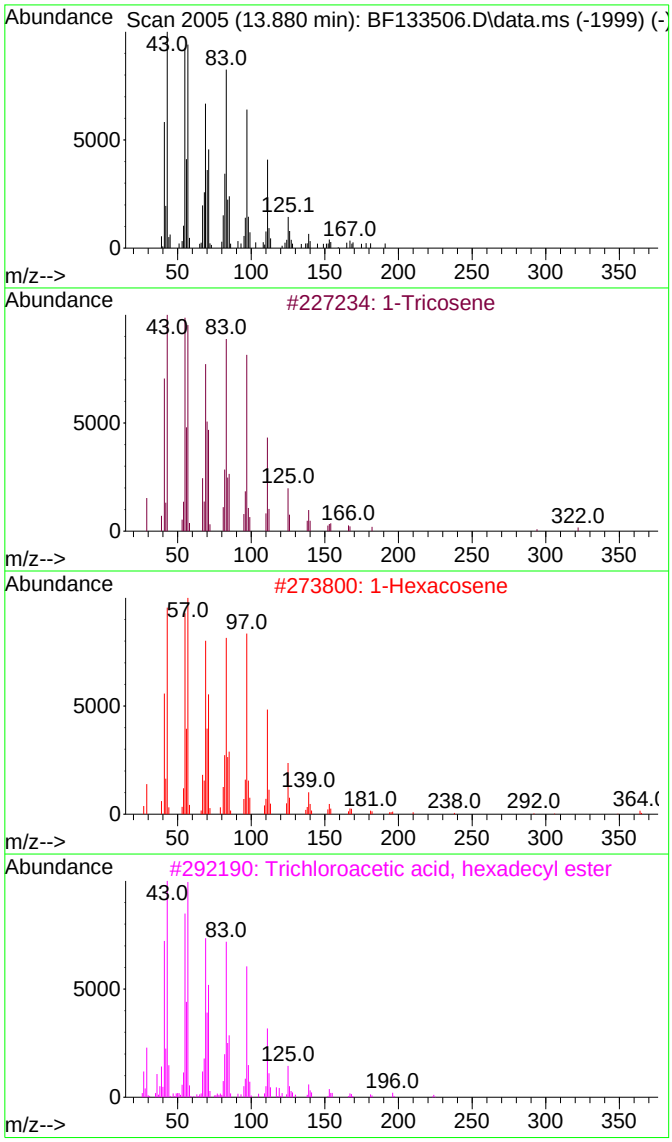
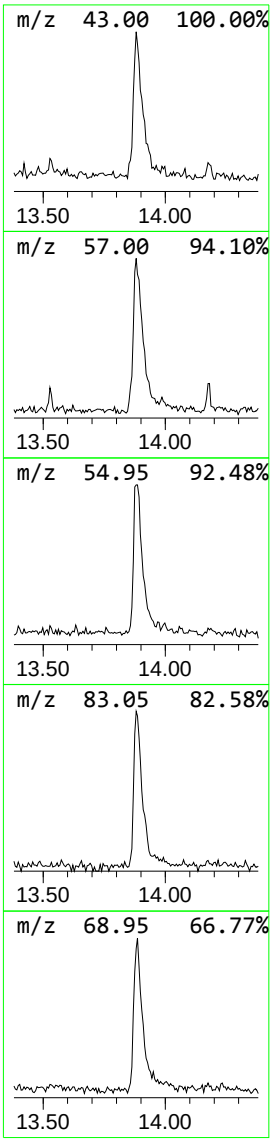
****

Peak Number 5 1-Tricosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.31 ng	218269	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	95
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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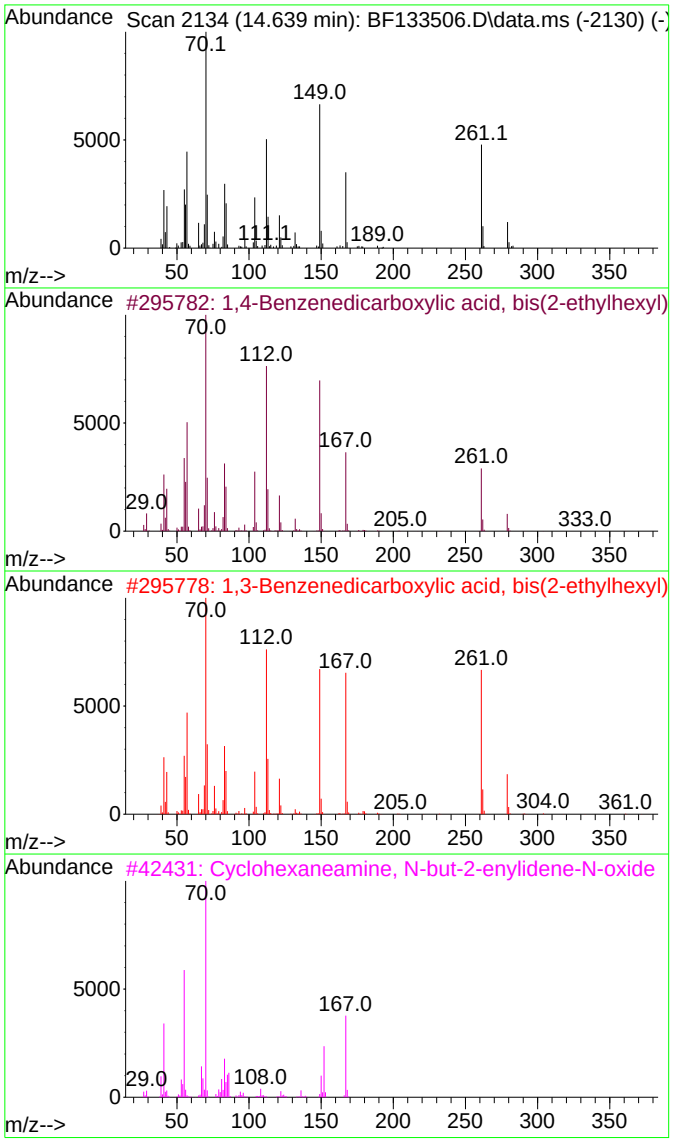
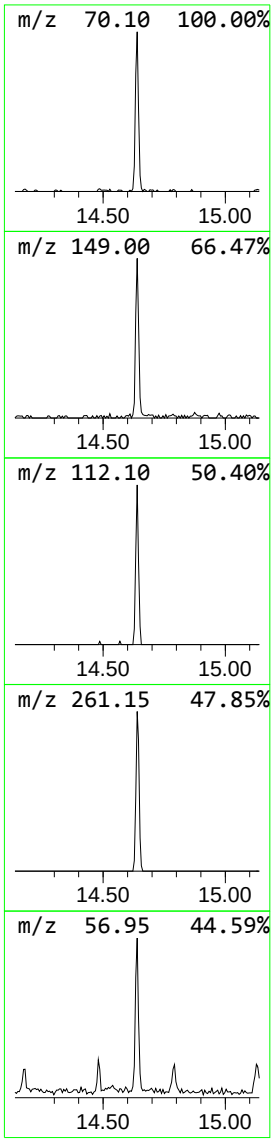
****
Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.639	2.49 ng	126109	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	70
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
3	Cyclohexaneamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	22
4	4-Nitrobenzoic acid, cyclobutyl ...	221	C11H11NO4	070335-00-1	16
5	Cyclohexanamine, N-methyl-	113	C7H15N	000100-60-7	14





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Hexen-2-one	4.416	2.6	ng	111149	1	6.834	842321	20.0
2-Pentanone, 4-...	5.040	22.3	ng	937579	1	6.834	842321	20.0
Benzophenone	10.586	9.0	ng	514118	3	9.875	1142790	20.0
n-Hexadecanoic ...	11.892	3.6	ng	214728	4	11.363	1190360	20.0
1-Tricosene	13.880	4.3	ng	218269	5	13.998	1013130	20.0
1,4-Benzenedica...	14.639	2.5	ng	126109	5	13.998	1013130	20.0