LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052623\
Data File : BF133508.D
Acq On : 26 May 2023 20:02
Operator : CG\JU
Sample : 02945-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TWP03

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: BF133508.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	13	rVB	1500019	1565189	39.03%	6.757%
2	2.222	19	23	31	rVB	65563	85424	2.13%	0.369%
3	4.422	393	397	404	rVB	70664	76150	1.90%	0.329%
4	5.045	498	503	506	rBV	1000012	1023492	25.52%	4.418%
5	5.445	566	571	574	rBV	1378853	1325766	33.06%	5.723%
6	5.851	636	640	644	rVB	51024	45320	1.13%	0.196%
7	6.451	737	742	745	rBV	934523	837267	20.88%	3.614%
8	6.834	804	807	811	rBV	1031633	817876	20.39%	3.531%
9	7.404	898	904	907	rBV	2532221	2518693	62.81%	10.873%
10	7.475	912	916	920	rVB	60667	59593	1.49%	0.257%
11	8.122	1022	1026	1029	rBV	1181404	1054820	26.30%	4.553%
12	9.198	1204	1209	1212	rBV	4548072	4010251	100.00%	17.312%
13	9.875	1320	1324	1327	rBV	1416809	1096888	27.35%	4.735%
14	10.586	1442	1445	1449	rBV	330831	262107	6.54%	1.131%
15	10.663	1453	1458	1461	rBV	1853221	1733822	43.23%	7.485%
16	11.357	1573	1576	1580	rBV	1235203	1134932	28.30%	4.899%
17	11.892	1663	1667	1671	rBV	181527	177638	4.43%	0.767%
18	12.680	1798	1801	1809	rBV	93860	100403	2.50%	0.433%
19	12.957	1843	1848	1851	rBV	3537309	3614556	90.13%	15.603%
20	13.874	2000	2004	2014	rVB	71417	107347	2.68%	0.463%
21	14.004	2022	2026	2029	rBV	853278	793443	19.79%	3.425%
22	15.462	2269	2274	2279	rBV	616843	724254	18.06%	3.126%

Sum of corrected areas: 23165231

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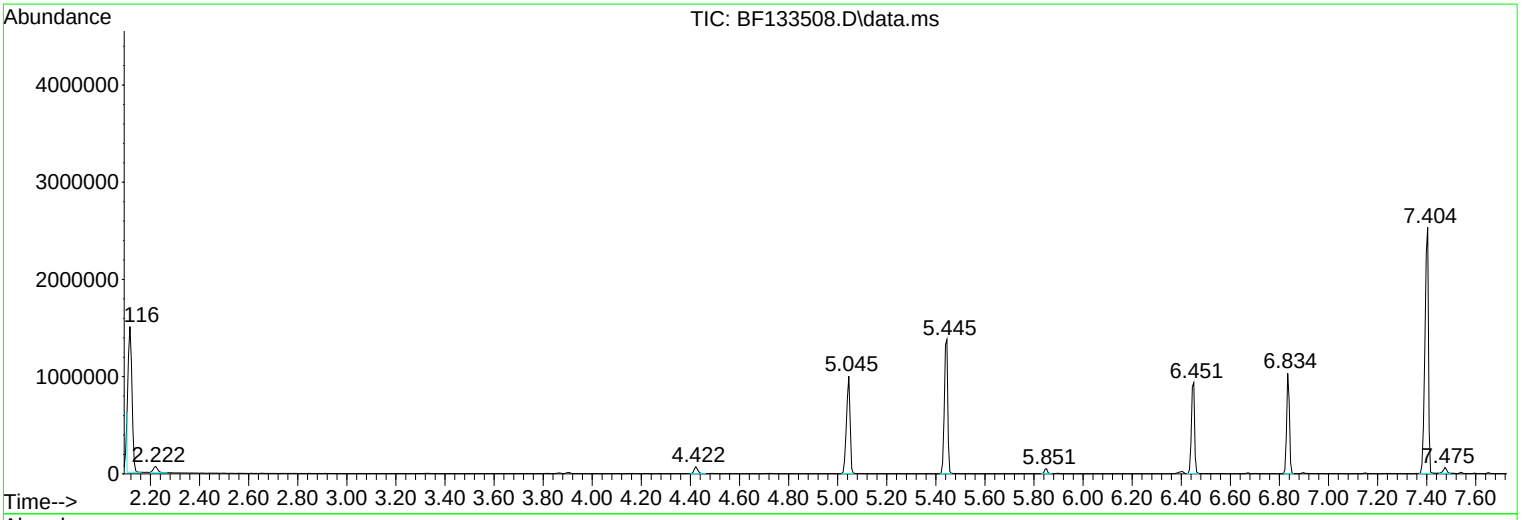
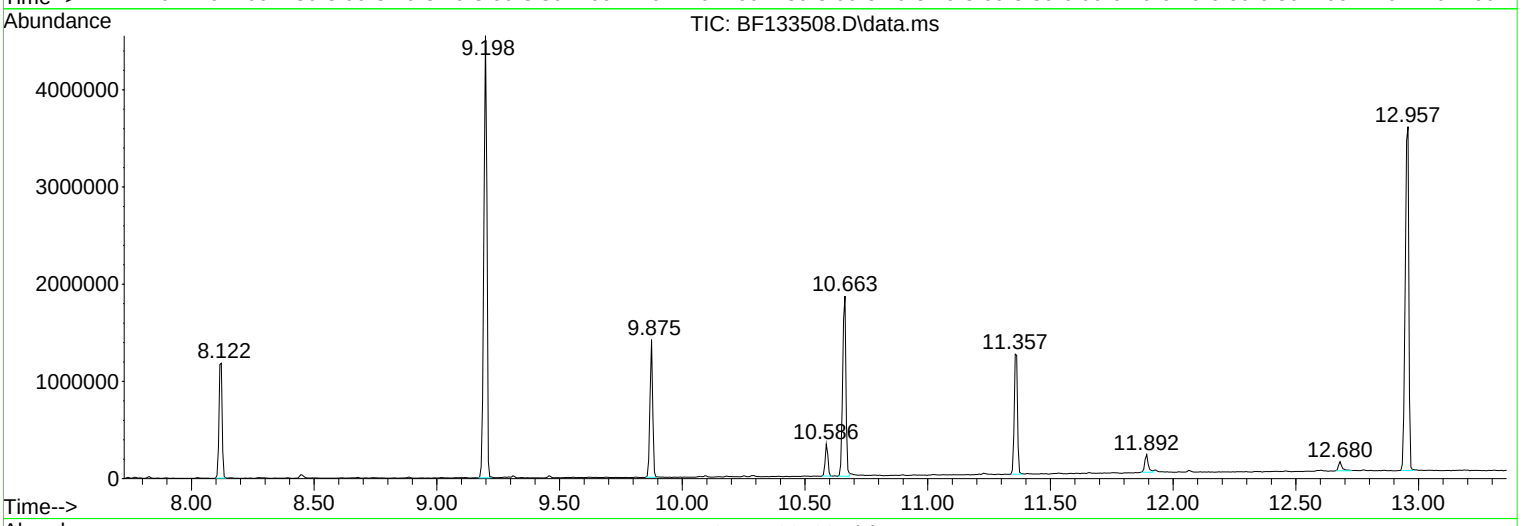
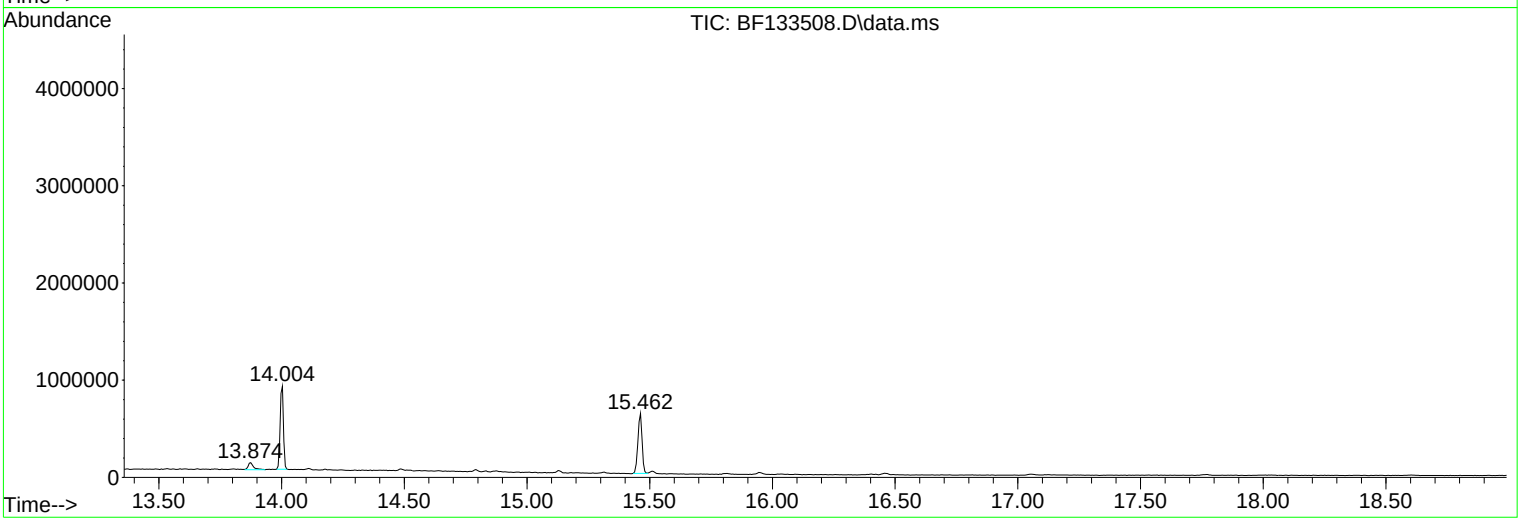
ClientSampleId :
TWP03

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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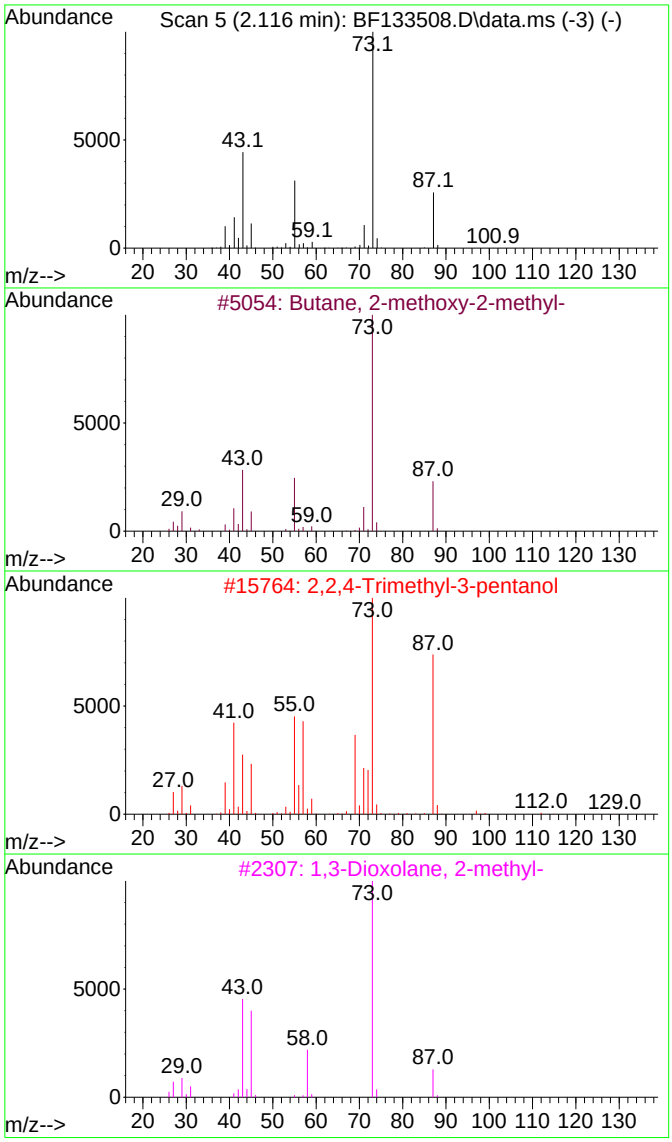
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

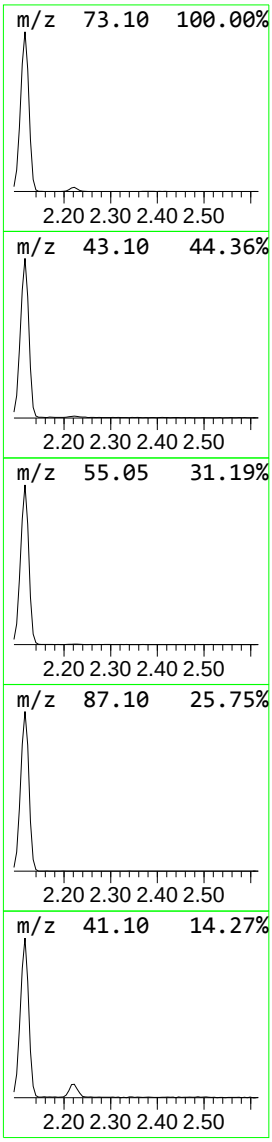
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	38.27 ng	1565190	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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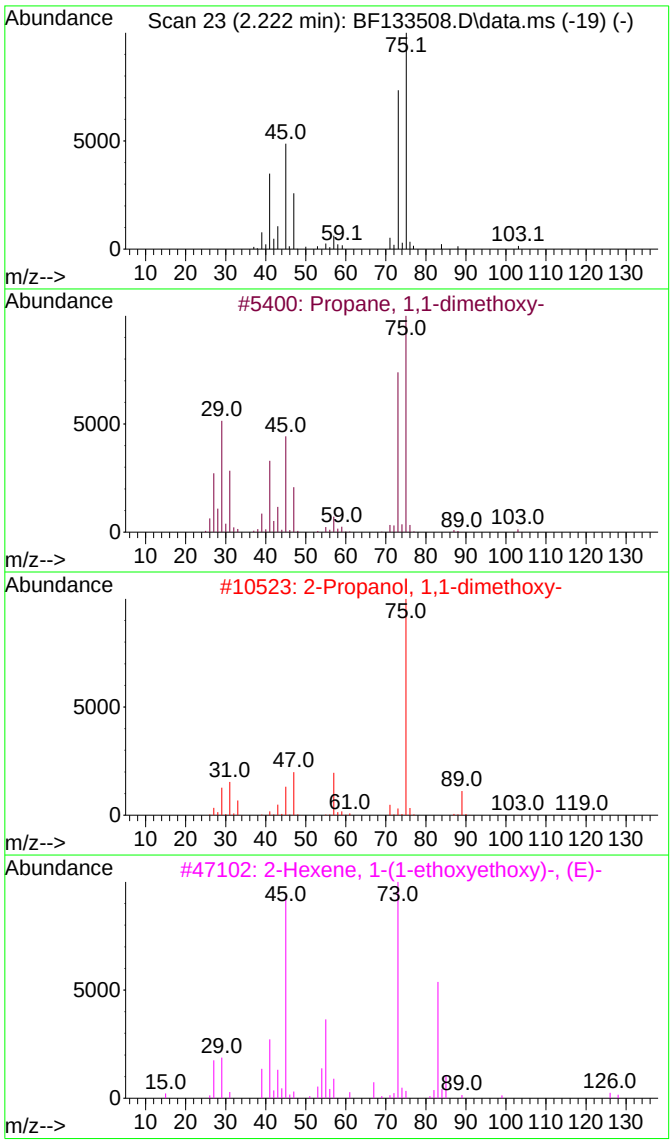
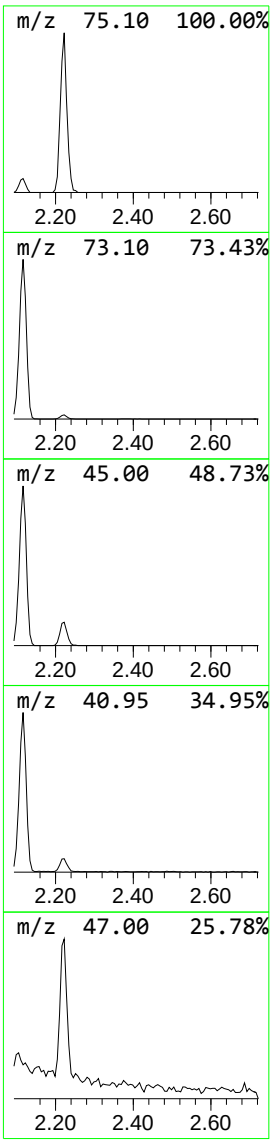
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	2.09 ng	85424	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	40
3	2-Hexene, 1-(1-ethoxyethoxy)-, (E)-	172	C10H20O2	054484-66-1	16
4	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	12
5	3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	10





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
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TIC Library : C:\Database\NIST20.L
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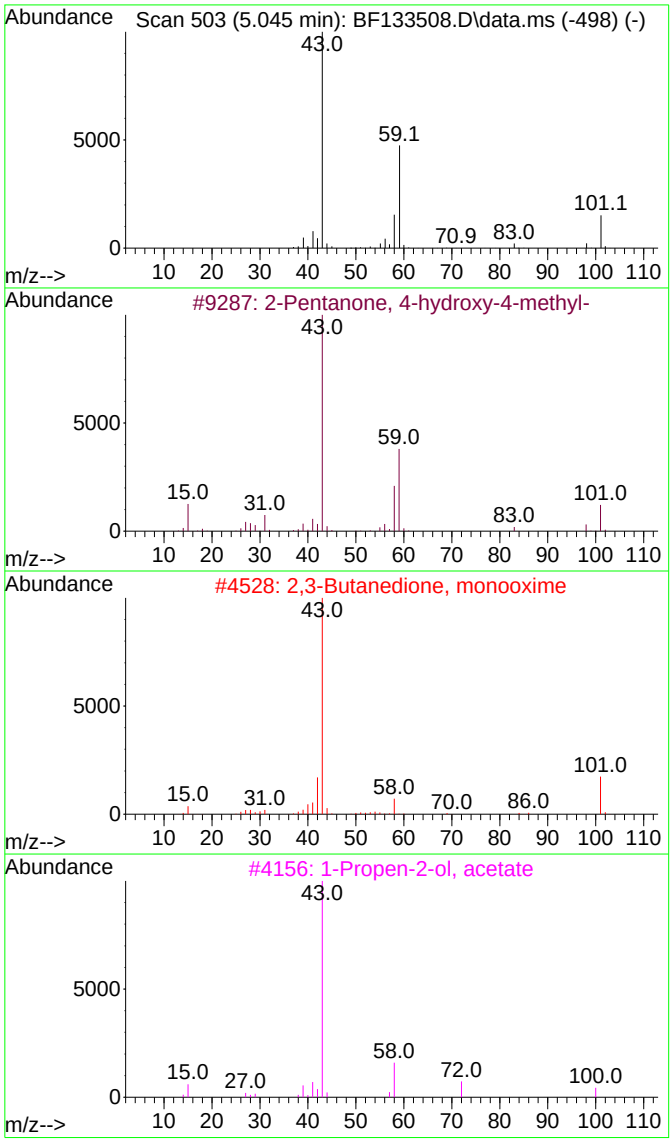
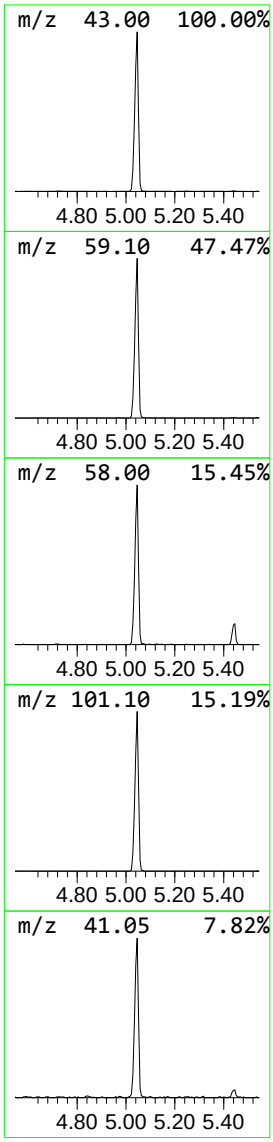
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	25.03 ng	1023490	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	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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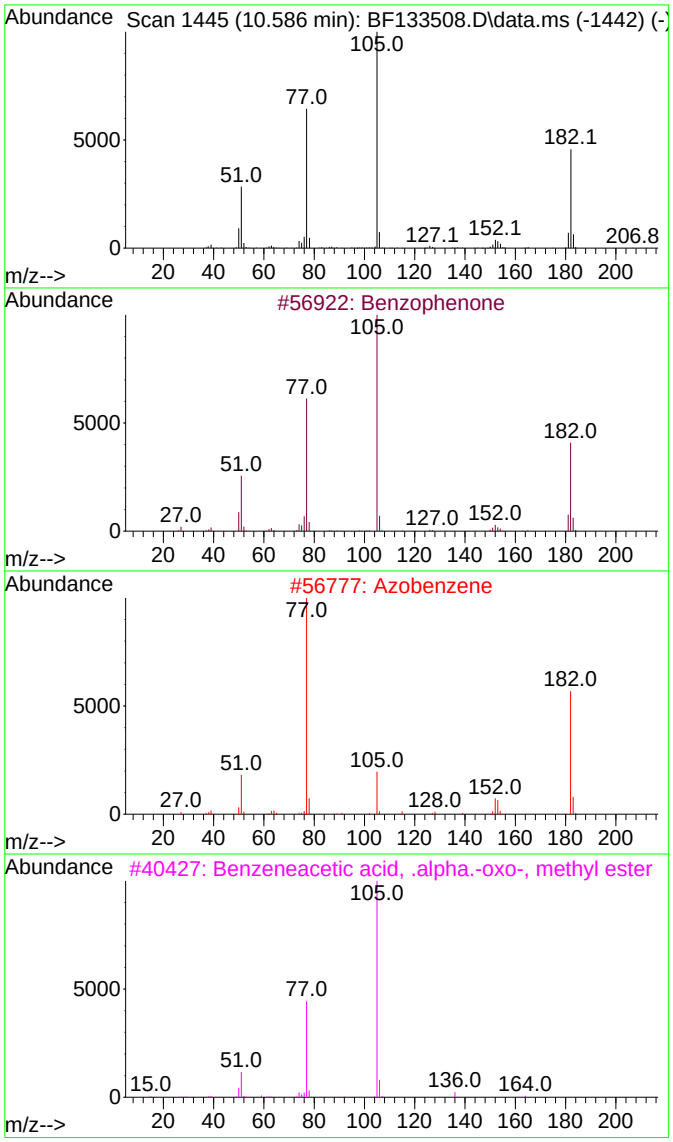
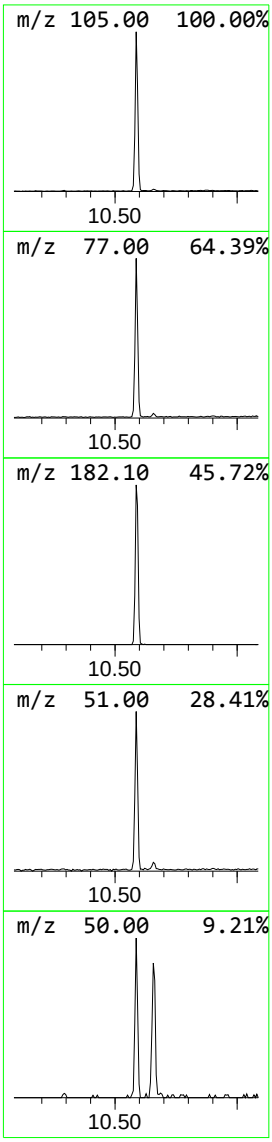
****

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	4.78 ng	262107	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	53
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	50
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	50
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50





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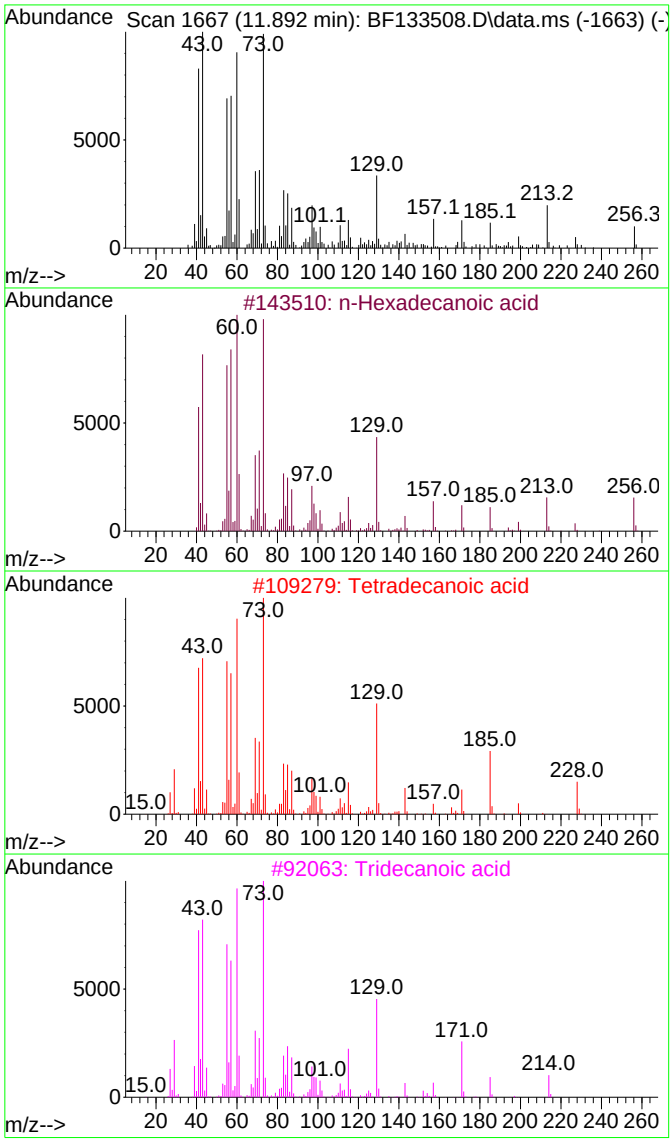
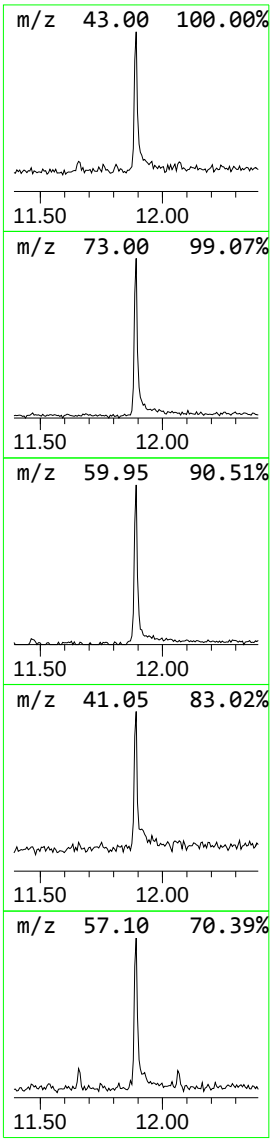
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	3.13 ng	177638	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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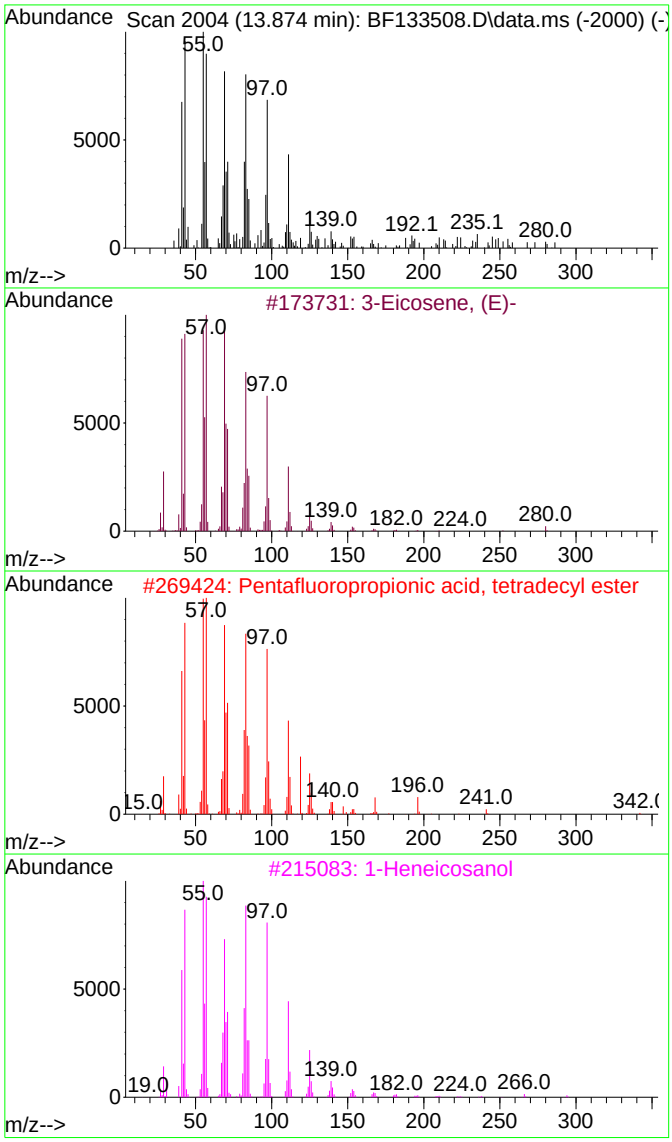
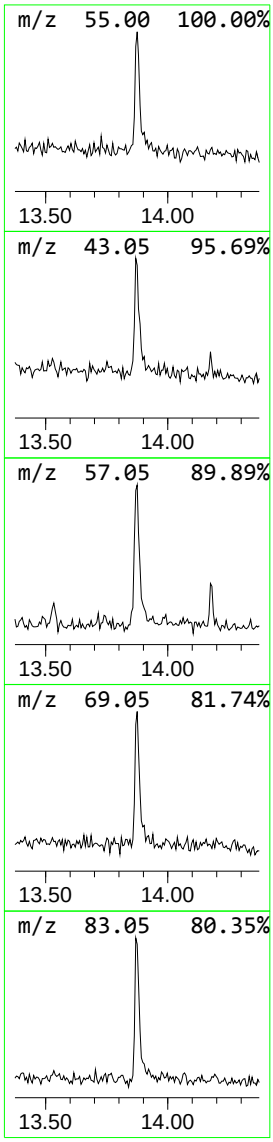
****

Peak Number 6 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.71 ng	107347	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	90





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.116	38.3	ng	1565190	1	6.834	817876	20.0
Propane, 1,1-di...	2.222	2.1	ng	85424	1	6.834	817876	20.0
2-Pentanone, 4-...	5.045	25.0	ng	1023490	1	6.834	817876	20.0
Benzophenone	10.586	4.8	ng	262107	3	9.875	1096890	20.0
n-Hexadecanoic ...	11.892	3.1	ng	177638	4	11.363	1134930	20.0
3-Eicosene, (E)-	13.874	2.7	ng	107347	5	14.004	793443	20.0