LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062121\
Data File : BF124397.D
Acq On : 21 Jun 2021 17:11
Operator : JU/CG
Sample : M2773-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124397.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	490	493	500	rBV	51562	65762	7.60%	1.163%
2	5.410	562	565	586	rBB	739991	661251	76.43%	11.697%
3	6.428	735	738	756	rBB	681659	627733	72.56%	11.104%
4	6.786	796	799	806	rBB	242813	208379	24.09%	3.686%
5	6.939	822	825	832	rBB	16644	21407	2.47%	0.379%
6	7.351	891	895	898	rBV	526659	438634	50.70%	7.759%
7	7.975	998	1001	1013	rBV	153144	154383	17.85%	2.731%
8	8.069	1013	1017	1026	rVB	313508	257905	29.81%	4.562%
9	9.145	1196	1200	1203	rBV	1155198	865121	100.00%	15.304%
10	9.263	1217	1220	1226	rVB	54473	46686	5.40%	0.826%
11	9.821	1312	1315	1319	rBV	375840	290451	33.57%	5.138%
12	10.616	1446	1450	1454	rBV	571184	497223	57.47%	8.796%
13	11.310	1565	1568	1572	rBV	356468	275897	31.89%	4.881%
14	11.704	1632	1635	1638	rBB	18874	14577	1.68%	0.258%
15	12.410	1752	1755	1760	rVB	55838	44794	5.18%	0.792%
16	12.898	1834	1838	1841	rBV	851981	683596	79.02%	12.093%
17	13.845	1994	1999	2002	rBV4	7696	16767	1.94%	0.297%
18	13.957	2014	2018	2022	rVB	203204	175174	20.25%	3.099%
19	15.056	2202	2205	2208	rVB3	10270	12278	1.42%	0.217%
20	15.415	2262	2266	2277	rVB	189928	233366	26.97%	4.128%
21	15.621	2296	2301	2306	rBV5	9684	15164	1.75%	0.268%
22	15.851	2337	2340	2344	rVB4	9039	11267	1.30%	0.199%
23	17.162	2557	2563	2569	rBV7	15761	35231	4.07%	0.623%

Sum of corrected areas: 5653046

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ClientSampleId :
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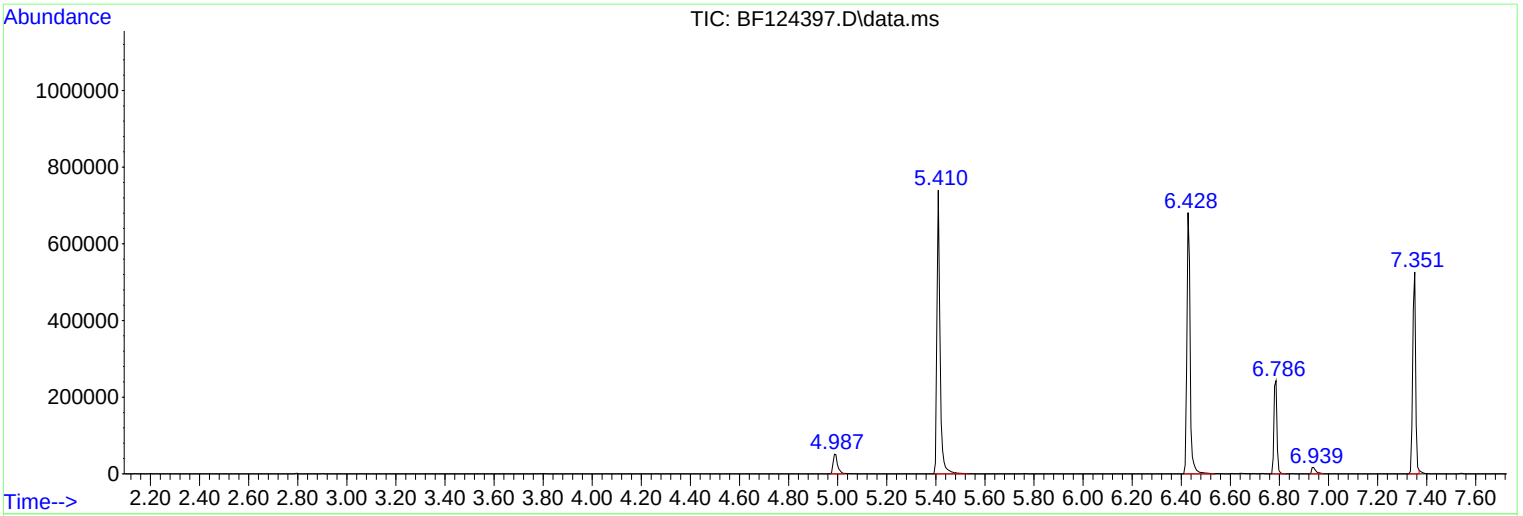
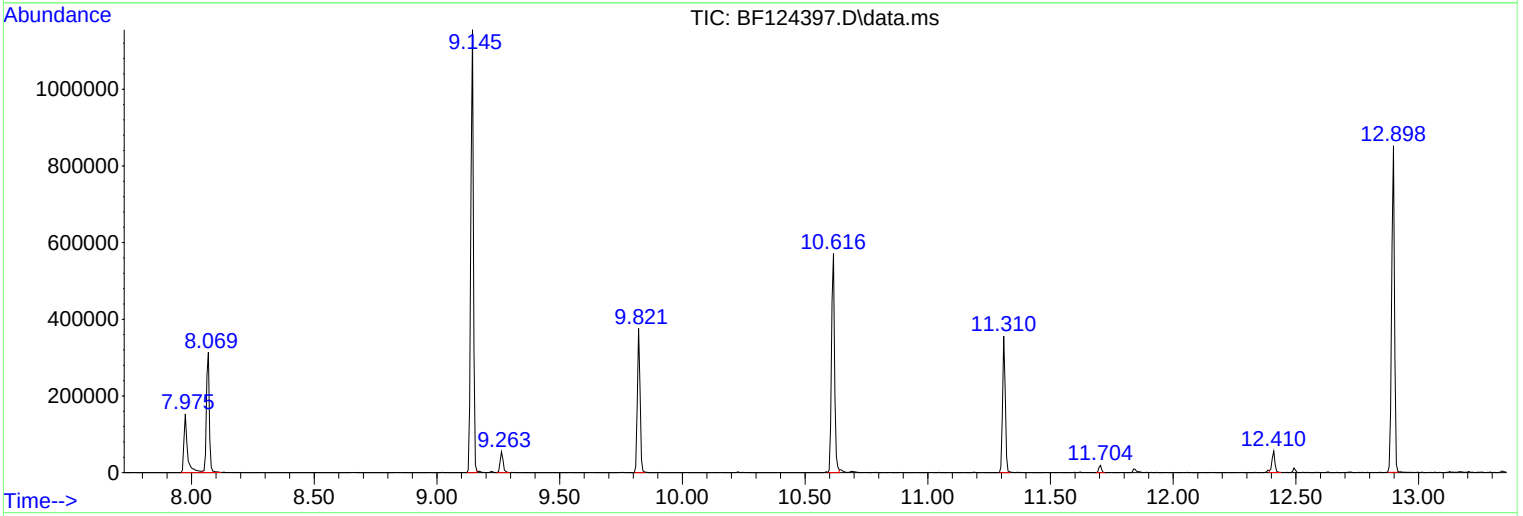
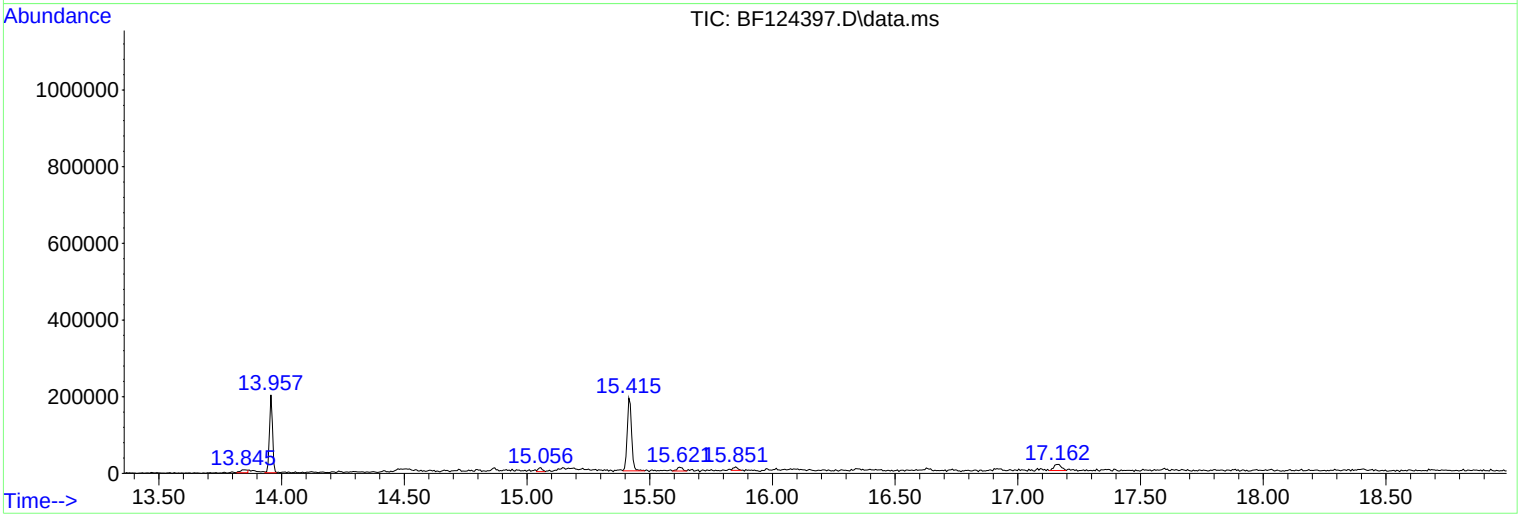
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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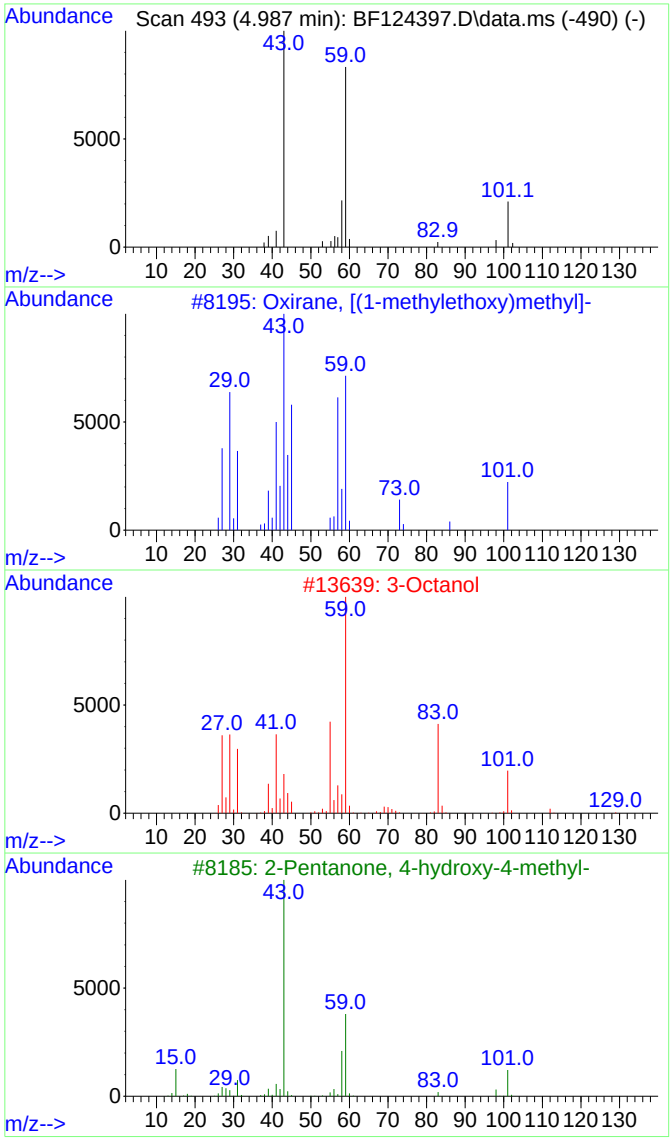
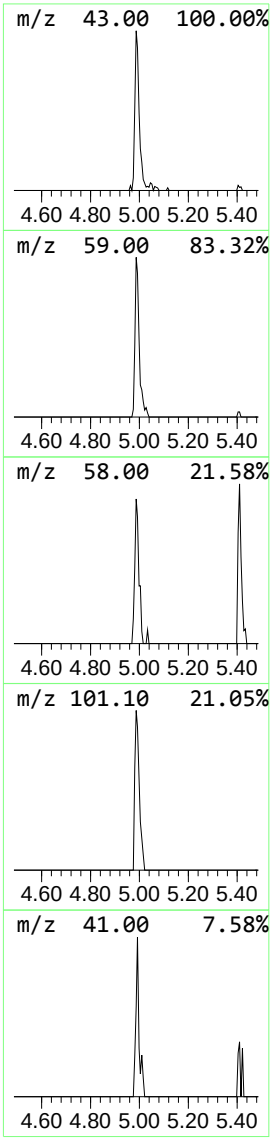
****
Peak Number 1 Oxirane, [(1-methylethoxy)m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	6.31 ng	65762	1,4-Dichlorobenzene-d4	6.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	64
2	3-Octanol	130	C8H18O	000589-98-0	36
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	23
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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BNA_F
ClientSampleId :
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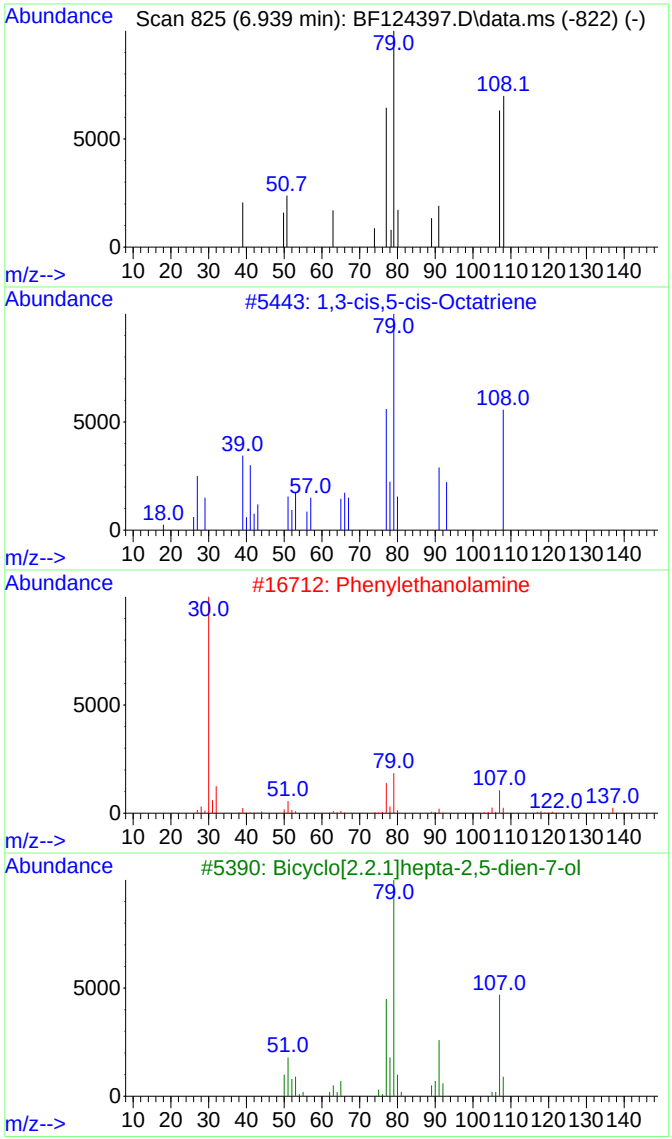
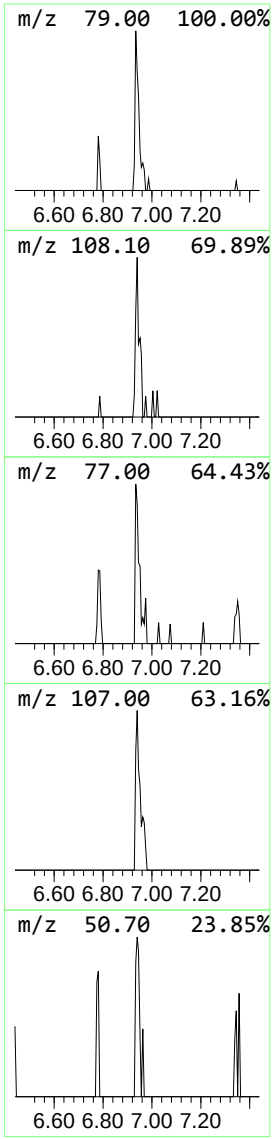
****

Peak Number 2 1,3-cis,5-cis-Octatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.939	2.05 ng	21407	1,4-Dichlorobenzene-d4	6.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-cis,5-cis-Octatriene	108	C8H12	040087-62-5	53
2	Phenylethanolamine	137	C8H11NO	007568-93-6	38
3	Bicyclo[2.2.1]hepta-2,5-dien-7-ol	108	C7H8O	000822-80-0	32
4	Benzene, nitroso-	107	C6H5NO	000586-96-9	27
5	3-Penten-1-yne, 3-methyl-	80	C6H8	001574-33-0	12





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Sample : M2773-07
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Instrument : BNA_F
ClientSampleId : SB-7

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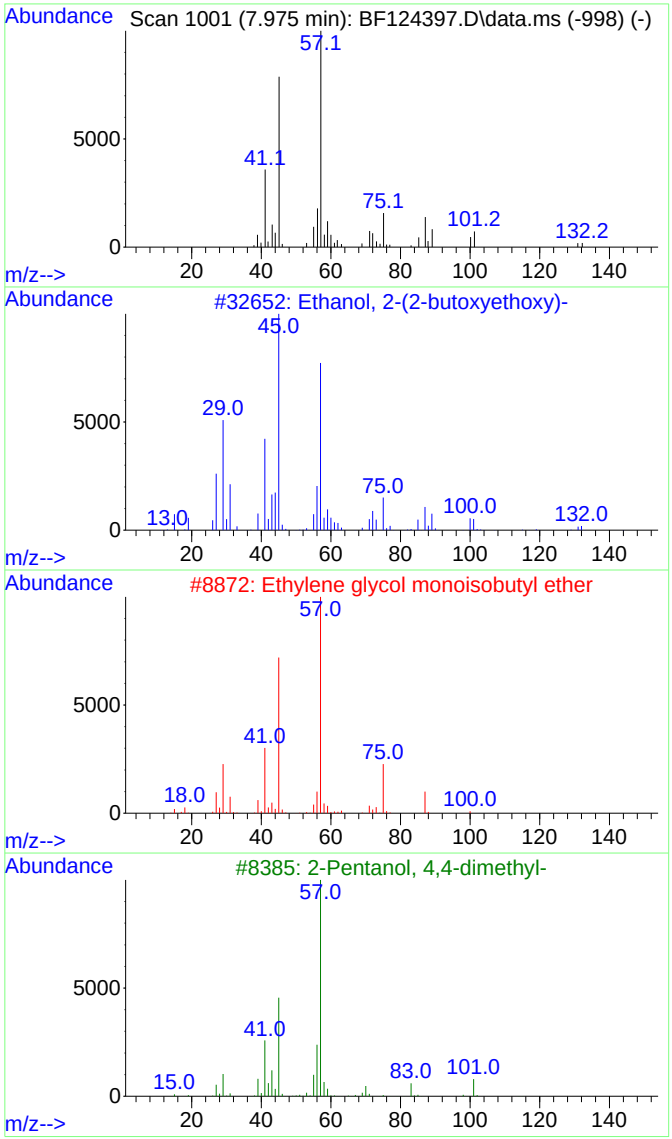
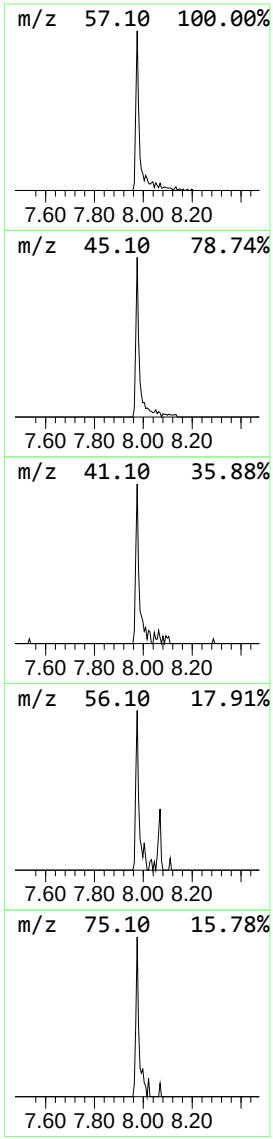
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.975	11.97 ng	154383	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	53
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	50
5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50





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Instrument : BNA_F
ClientSampleId : SB-7

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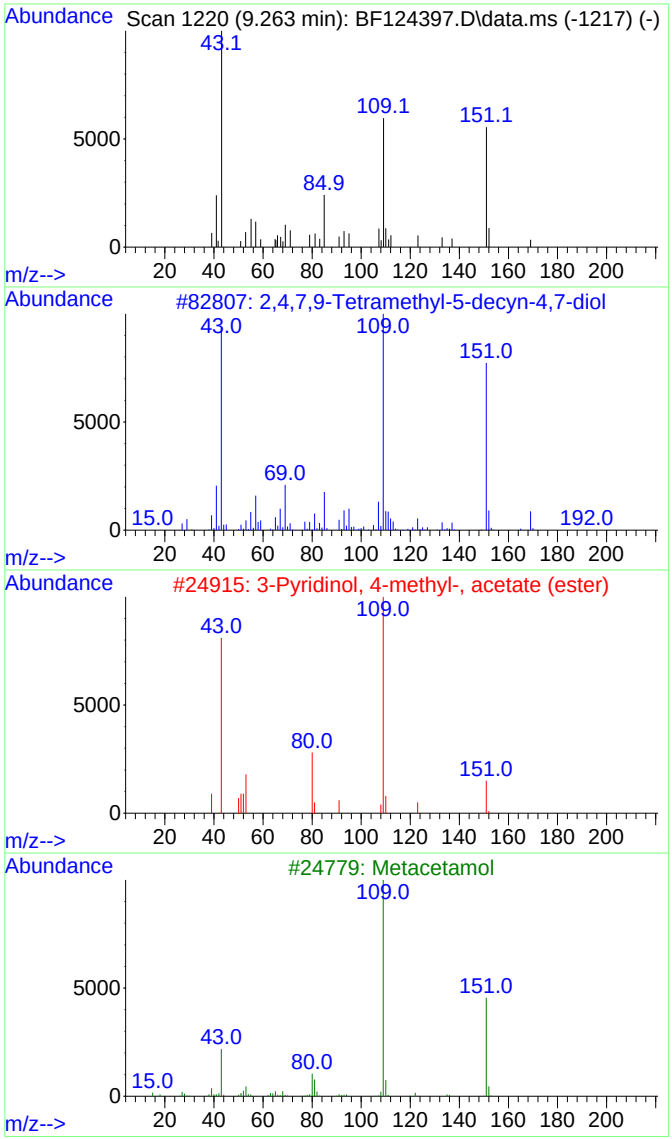
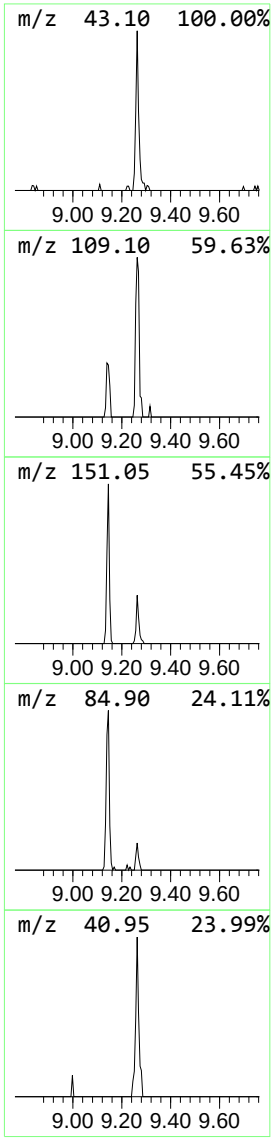
****
Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.263	3.21 ng	46686	Acenaphthene-d10	9.821

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	72
2	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	50
3	Metacetamol	151	C8H9NO2	000621-42-1	49
4	(7,7-Dimethyl-2-oxobicyclo[2.2.1...	250	C10H15ClO3S	1000194-76-1	38
5	Acetaminophen	151	C8H9NO2	000103-90-2	38





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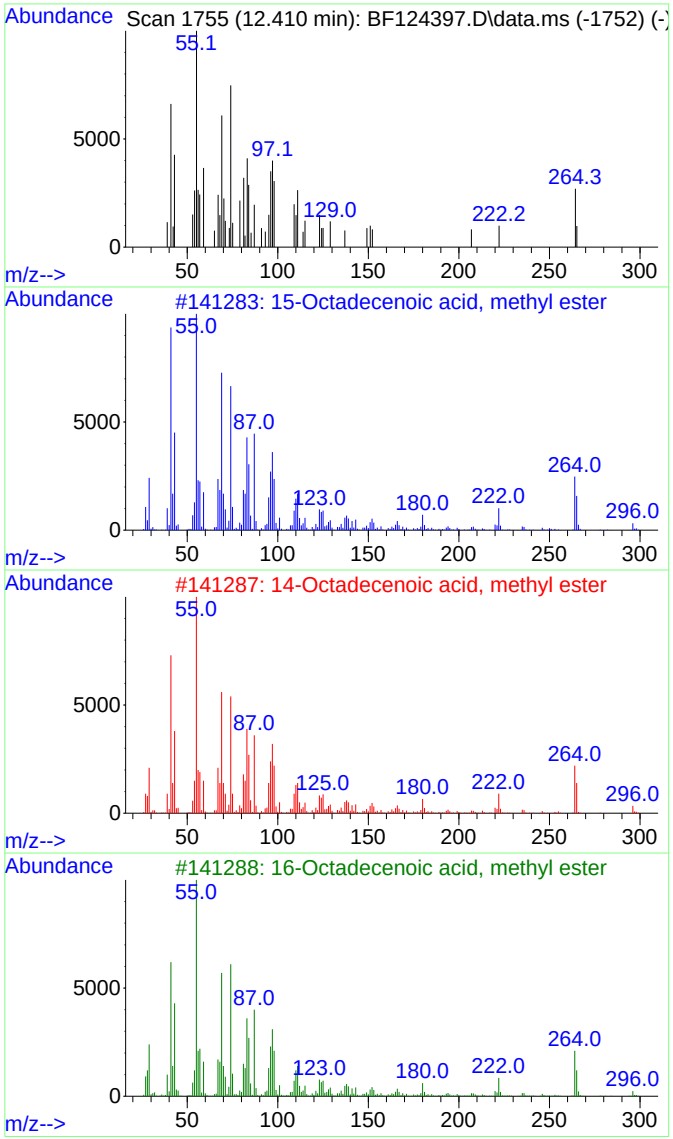
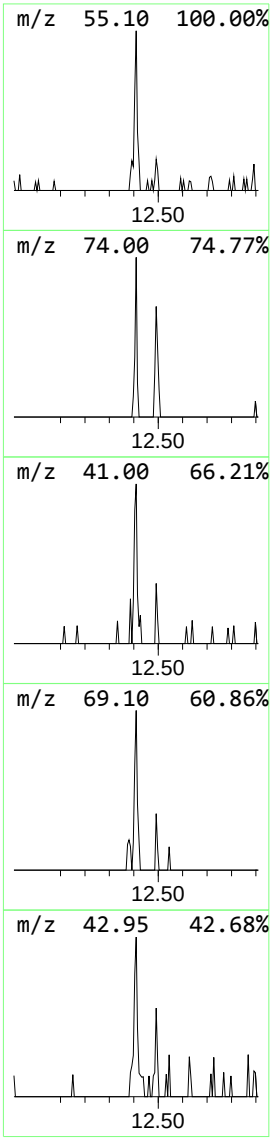
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 15-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	3.25 ng	44794	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	68
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	64
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	64
4	9-Dodecenoic acid, methyl ester,...	212	C13H24O2	055030-26-7	53
5	Oxiraneundecanoic acid, 3-pentyl...	312	C19H36O3	038520-31-9	53





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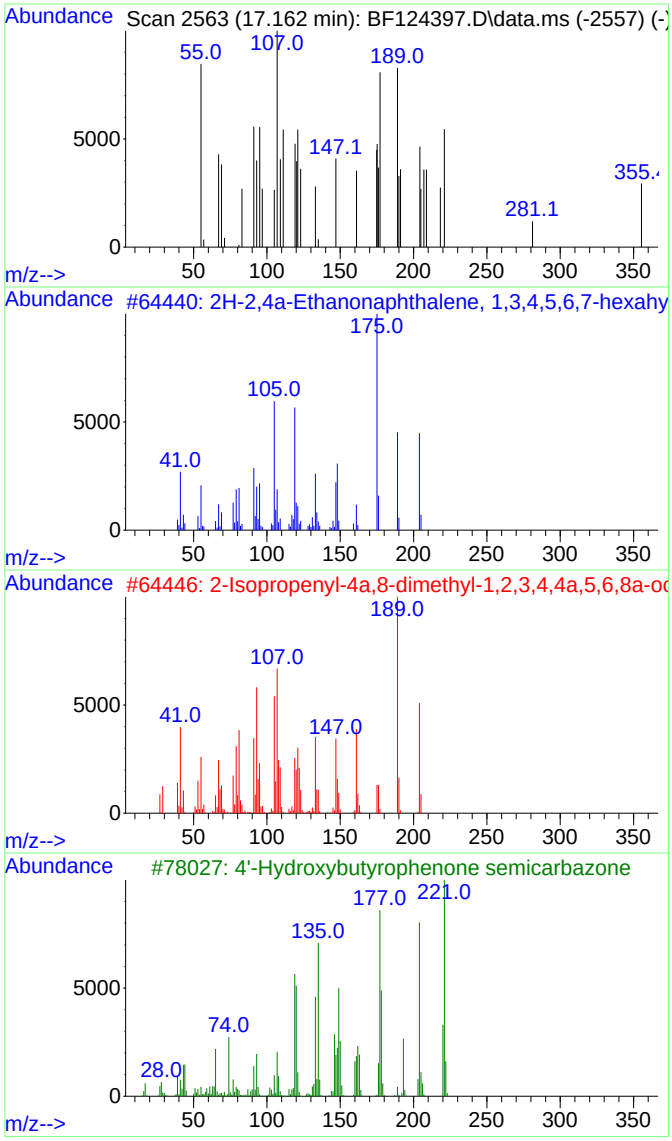
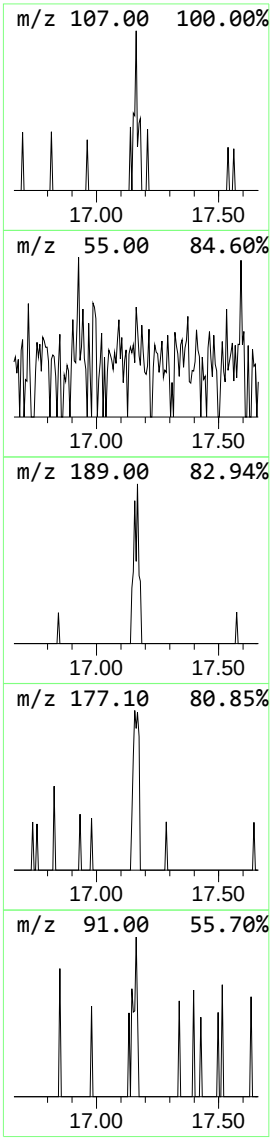
****

Peak Number 6 unknown17.162 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.162	3.02 ng	35231	Perylene-d12	15.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-2,4a-Ethanonaphthalene, 1,3,4...	204	C15H24	032391-44-9	27
2	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	25
3	4'-Hydroxybutyrophenone semicarb...	221	C11H15N3O2	1000240-11-4	22
4	Cyclopropa[d]naphthalen-2(4aH)-o...	204	C14H20O	004677-90-1	22
5	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	16





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Oxirane, [(1-me...	4.987	6.3	ng	65762	1	6.786	208379	20.0
1,3-cis,5-cis-O...	6.939	2.0	ng	21407	1	6.786	208379	20.0
Ethanol, 2-(2-b...	7.975	12.0	ng	154383	2	8.069	257905	20.0
2,4,7,9-Tetrame...	9.263	3.2	ng	46686	3	9.821	290451	20.0
15-Octadecenoic...	12.410	3.3	ng	44794	4	11.310	275897	20.0
unknown17.162	17.162	3.0	ng	35231	6	15.415	233366	20.0