LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
Data File : BF107636.D
Acq On : 24 Jul 2018 23:01
Operator : JU/SJ
Sample : J4011-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20180415-COMPOSITE-1

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-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.207	484	488	507	rBV	567029	725510	18.34%	1.981%
2	5.607	552	556	581	rBV	2601055	3729602	94.29%	10.181%
3	6.607	721	726	745	rBV	2542295	3836675	96.99%	10.473%
4	6.742	745	749	773	rVB	3476038	3939857	99.60%	10.755%
5	6.966	784	787	804	rBV	1024937	1320160	33.37%	3.604%
6	7.125	810	814	842	rVB	2879407	3077868	77.81%	8.402%
7	7.531	879	883	894	rBV	1941869	2242152	56.68%	6.121%
8	8.248	1001	1005	1025	rBV	1430663	1689598	42.71%	4.612%
9	9.325	1182	1188	1203	rBV	4022150	3955630	100.00%	10.798%
10	9.425	1203	1205	1222	rVB7	33391	76894	1.94%	0.210%
11	9.713	1251	1254	1261	rBV	480164	467944	11.83%	1.277%
12	10.013	1301	1305	1308	rBV	1500023	1508270	38.13%	4.117%
13	10.042	1308	1310	1323	rVB	141408	162286	4.10%	0.443%
14	10.419	1372	1374	1377	rVB	56165	43045	1.09%	0.118%
15	10.801	1435	1439	1452	rBV	1759908	2021524	51.10%	5.518%
16	10.895	1452	1455	1461	rVB	58776	76497	1.93%	0.209%
17	11.507	1555	1559	1567	rBV	1300682	1431186	36.18%	3.907%
18	12.007	1641	1644	1656	rBV	160308	209168	5.29%	0.571%
19	12.719	1762	1765	1769	rBV	119619	129555	3.28%	0.354%
20	12.795	1775	1778	1784	rBV7	24974	40163	1.02%	0.110%
21	12.954	1799	1805	1811	rBV2	99234	137640	3.48%	0.376%
22	13.089	1824	1828	1838	rBV	3054637	2916488	73.73%	7.961%
23	13.277	1858	1860	1866	rVB5	46111	78486	1.98%	0.214%
24	13.636	1918	1921	1926	rBV3	45864	54360	1.37%	0.148%
25	13.966	1974	1977	1982	rBV	148673	156516	3.96%	0.427%
26	14.154	2005	2009	2018	rBV	1227085	1306082	33.02%	3.565%
27	14.289	2029	2032	2035	rVB	54683	52335	1.32%	0.143%
28	14.589	2081	2083	2091	rVB	81301	95039	2.40%	0.259%
29	14.913	2136	2138	2141	rVB	97178	85326	2.16%	0.233%
30	14.995	2149	2152	2156	rVB	80782	85989	2.17%	0.235%
31	15.689	2264	2270	2279	rBV	631064	980771	24.79%	2.677%

Sum of corrected areas: 36632616

LSC Report - Integrated Chromatogram

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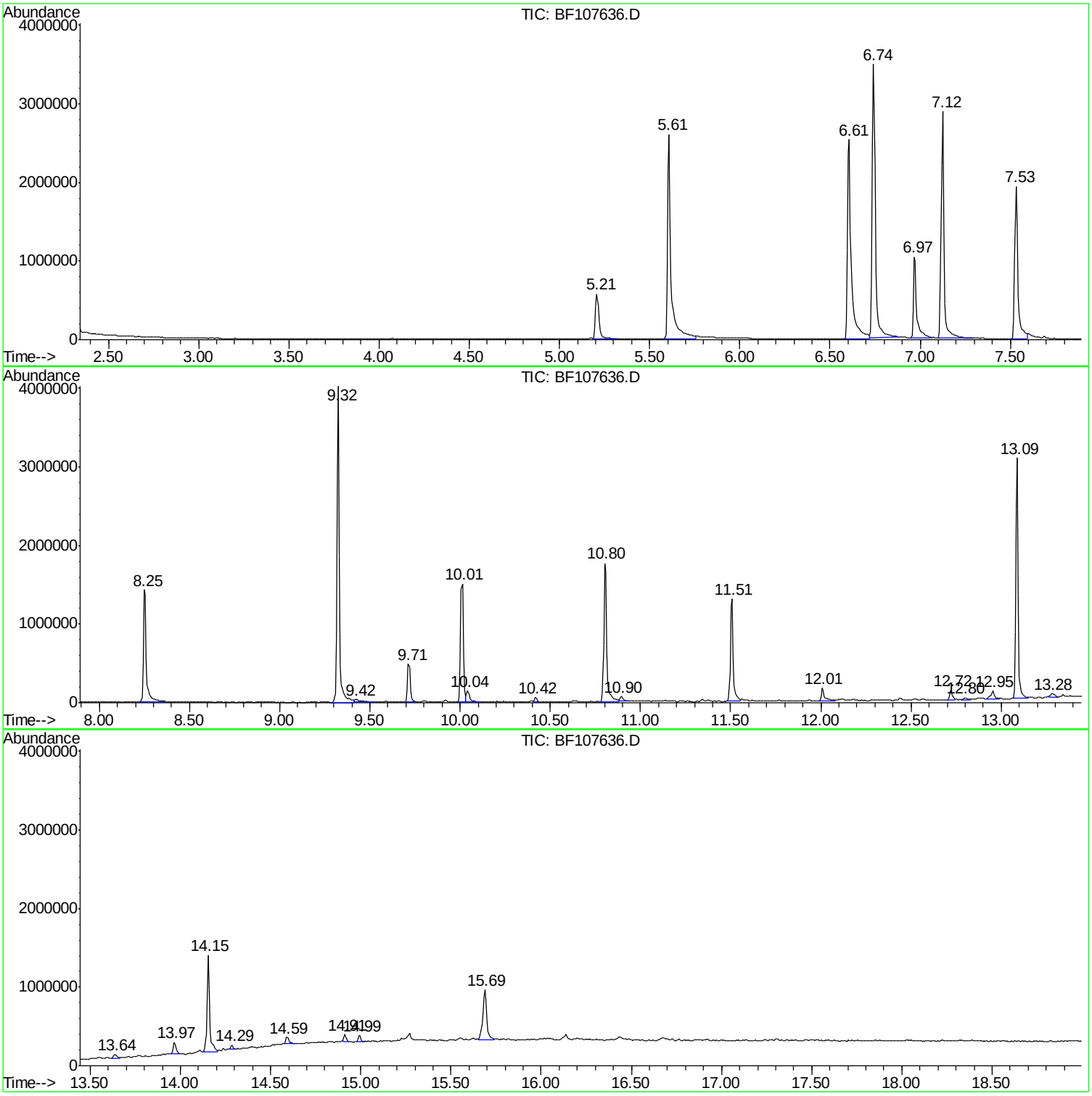
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20180415-COMPOSITE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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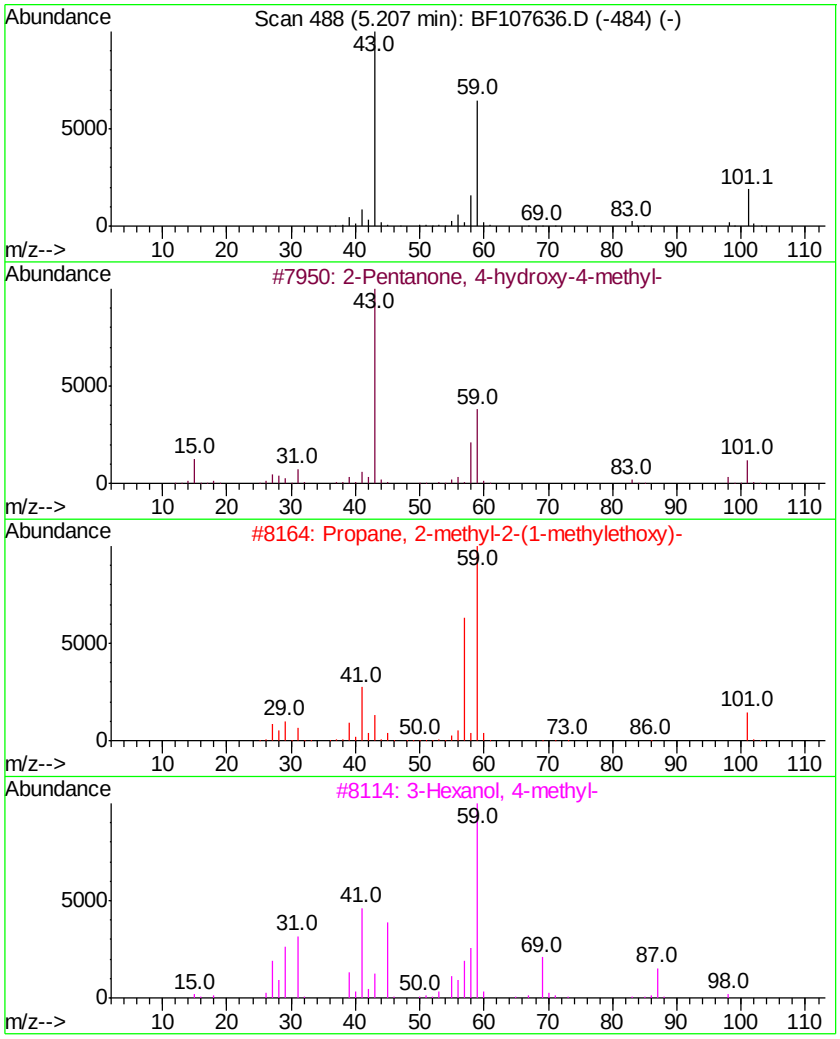
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

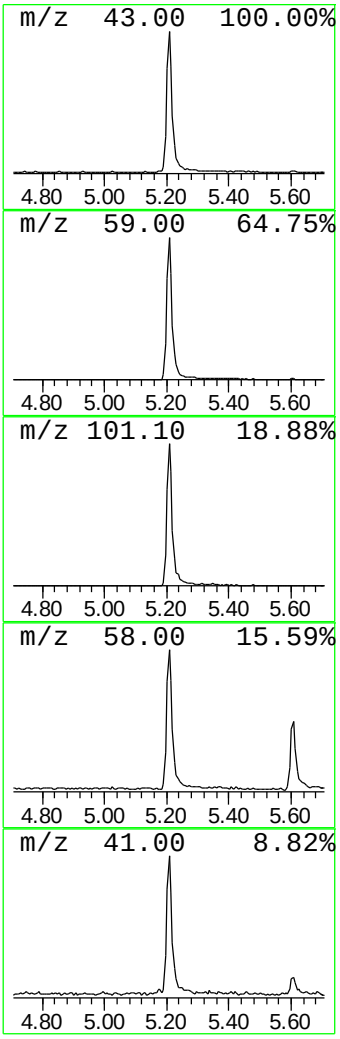
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	10.99 ng	725510	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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BNA_F
ClientSampleId :
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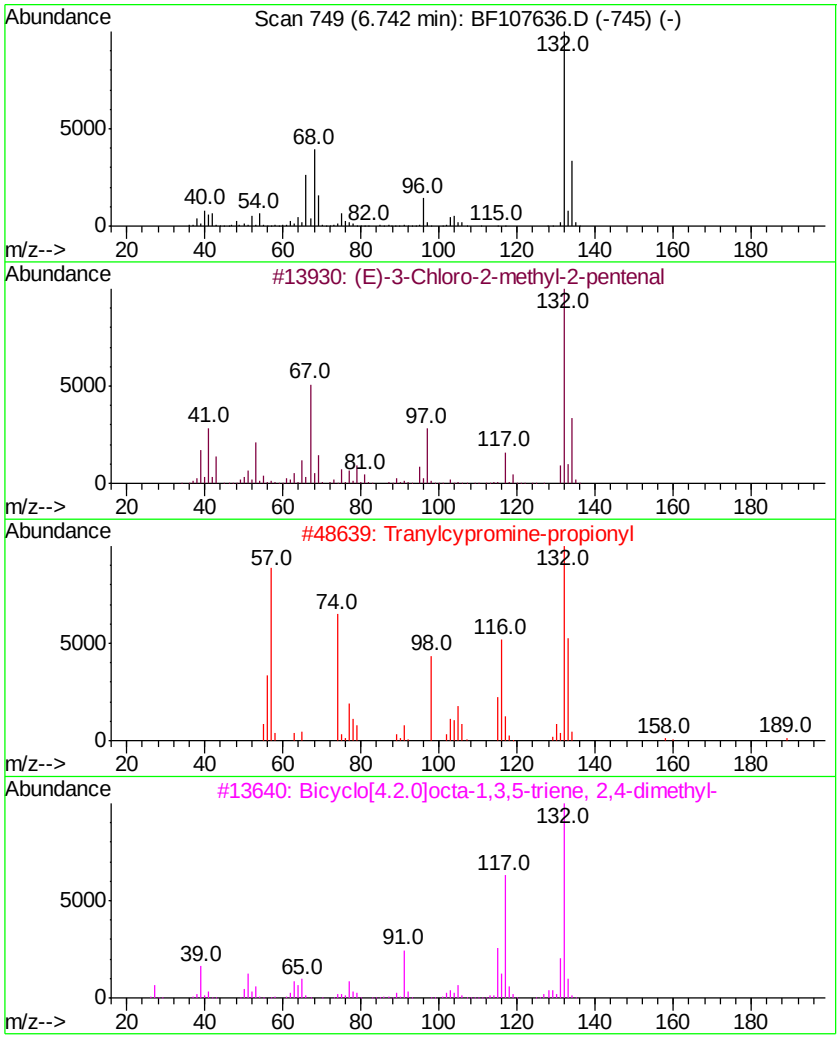
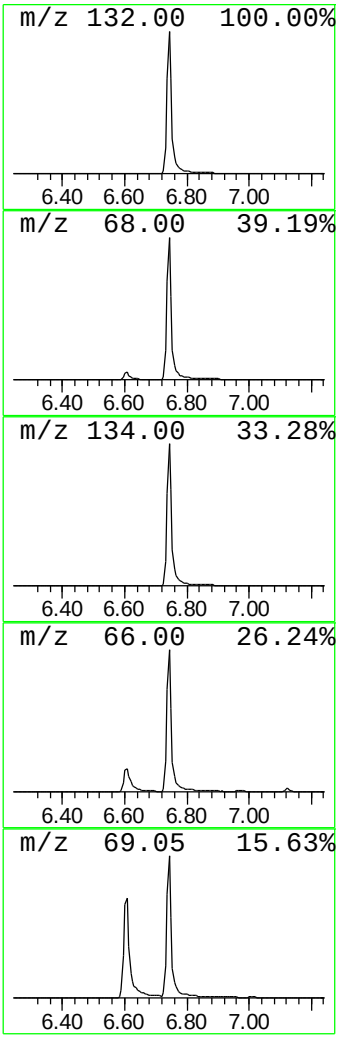
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	59.69 ng	3939860	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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BNA_F
ClientSampleId :
20180415-COMPOSITE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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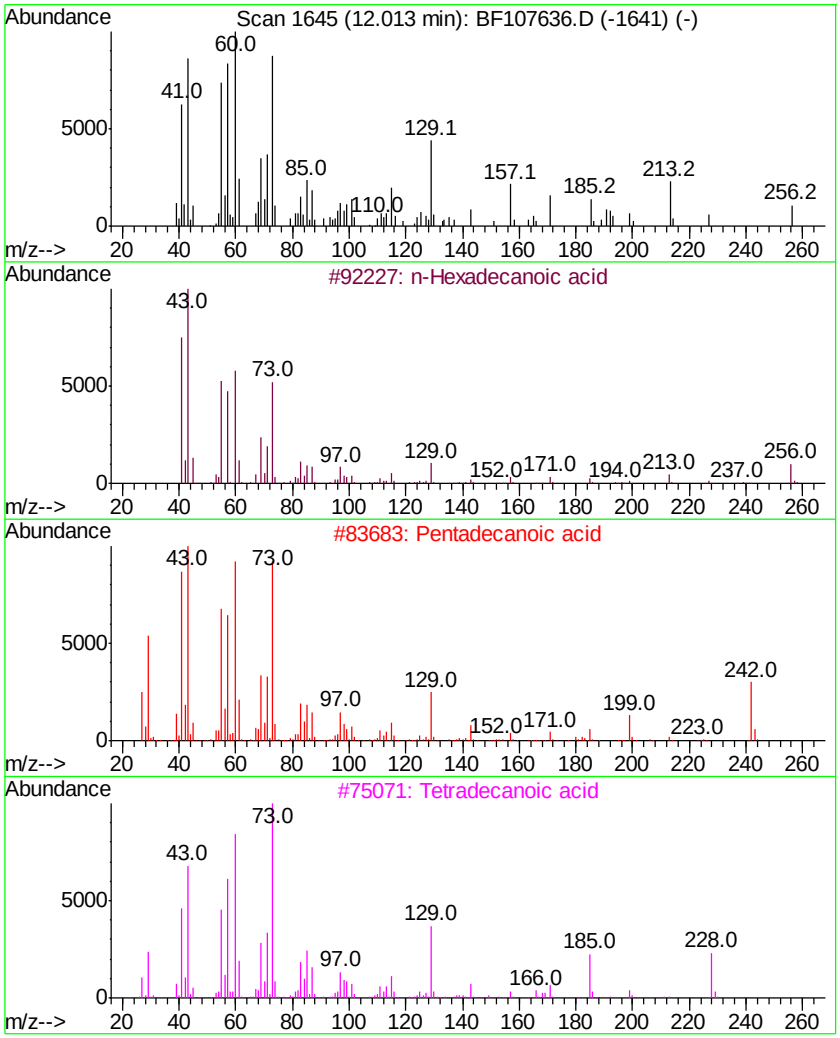
TIC Integration Parameters: LSCINT.P

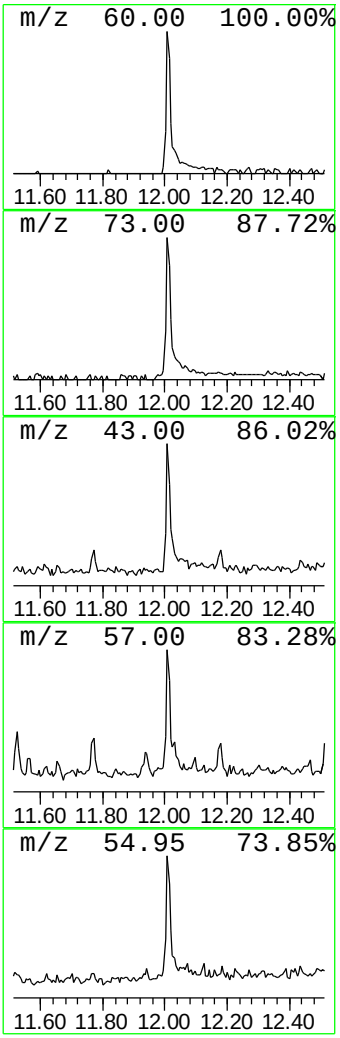
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.92 ng	209168	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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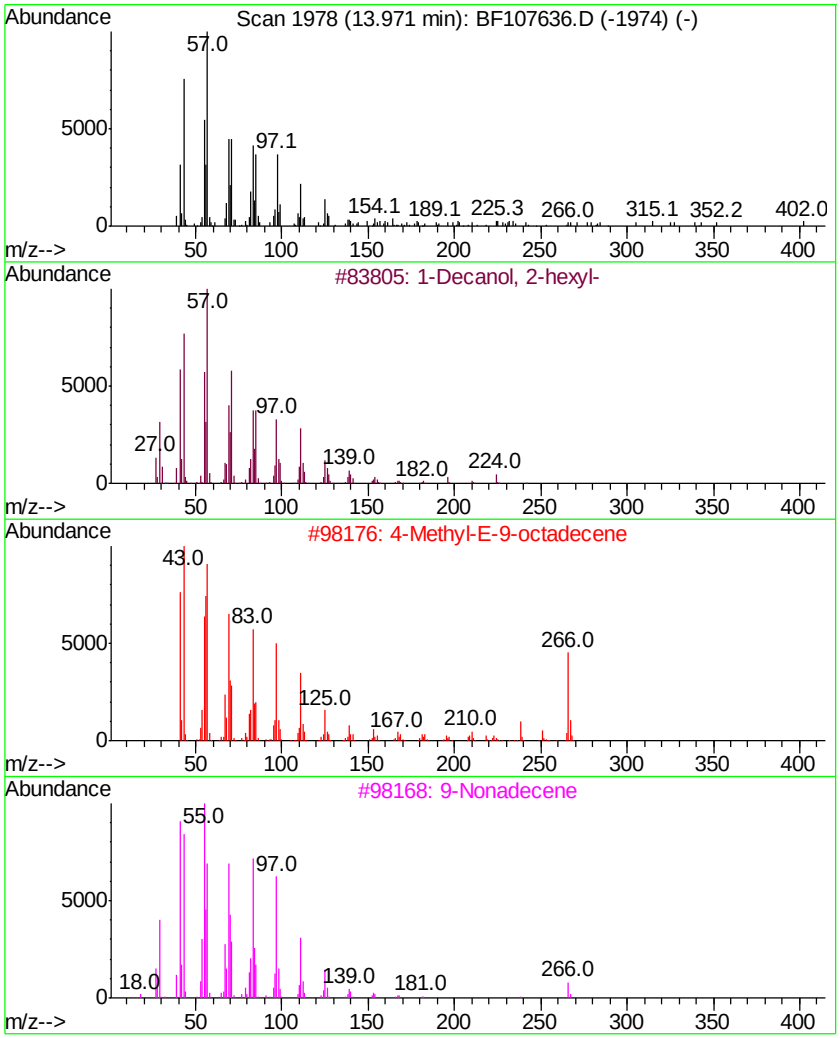
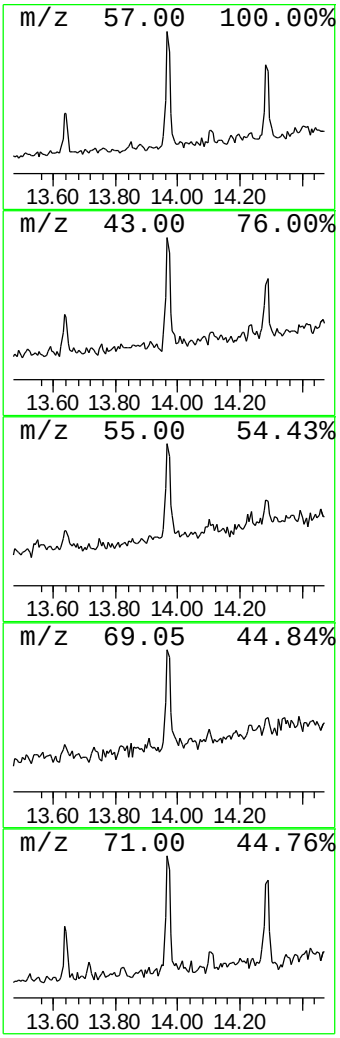
****

Peak Number 6 1-Decanol, 2-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.40 ng	156516	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	86
2	4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	86
3	9-Nonadecene	266	C19H38	031035-07-1	83
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	64
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	62





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	11.0	ng	725510	1	6.97	1320160	20.0
unknown6.74	6.74	59.7	ng	3939860	1	6.97	1320160	20.0
n-Hexadecanoic acid	12.01	2.9	ng	209168	4	11.51	1431190	20.0
1-Decanol, 2-hexyl-	13.97	2.4	ng	156516	5	14.15	1306080	20.0