LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091812.D
Acq On : 20 Dec 2016 11:36
Operator : UM/SJ
Sample : H6147-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-10

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:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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	4.247	187	189	193	rBV	73568	99334	1.45%	0.208%
2	4.921	246	248	251	rBV	862143	1100054	16.01%	2.307%
3	5.367	284	287	289	rBV	3068857	3250861	47.32%	6.817%
4	6.407	375	378	380	rBV	2196396	2148345	31.27%	4.505%
5	6.533	386	389	391	rBV	5178362	5390897	78.48%	11.304%
6	6.762	406	409	411	rBV	946111	1122234	16.34%	2.353%
7	6.910	420	422	425	rVB	3307086	4654460	67.76%	9.760%
8	7.322	455	458	461	rBV	2761337	3865542	56.27%	8.106%
9	8.042	518	521	524	rBV	1671881	1517646	22.09%	3.182%
10	9.128	613	616	618	rBV	5769487	6869479	100.00%	14.404%
11	9.516	648	650	653	rBV	200713	176943	2.58%	0.371%
12	9.790	672	674	677	rBV	1547695	1660766	24.18%	3.482%
13	10.316	718	720	723	rBV	88923	104114	1.52%	0.218%
14	10.591	740	744	746	rBV	3142130	4166719	60.66%	8.737%
15	10.705	752	754	758	rVB	68156	75942	1.11%	0.159%
16	11.276	801	804	806	rBV	1939525	1701928	24.78%	3.569%
17	11.493	821	823	826	rBV	46402	73280	1.07%	0.154%
18	11.745	842	845	848	rBV5	51274	171441	2.50%	0.359%
19	11.825	849	852	856	rVV2	123350	298190	4.34%	0.625%
20	12.602	918	920	922	rBV	156725	199291	2.90%	0.418%
21	12.694	926	928	932	rBV2	130367	175890	2.56%	0.369%
22	12.865	940	943	946	rBV	5524168	6089896	88.65%	12.770%
23	13.768	1019	1022	1027	rVB2	114879	168421	2.45%	0.353%
24	13.905	1032	1034	1037	rBV	1259002	1465053	21.33%	3.072%
25	15.311	1154	1157	1160	rBV	921880	1143607	16.65%	2.398%

Sum of corrected areas: 47690333

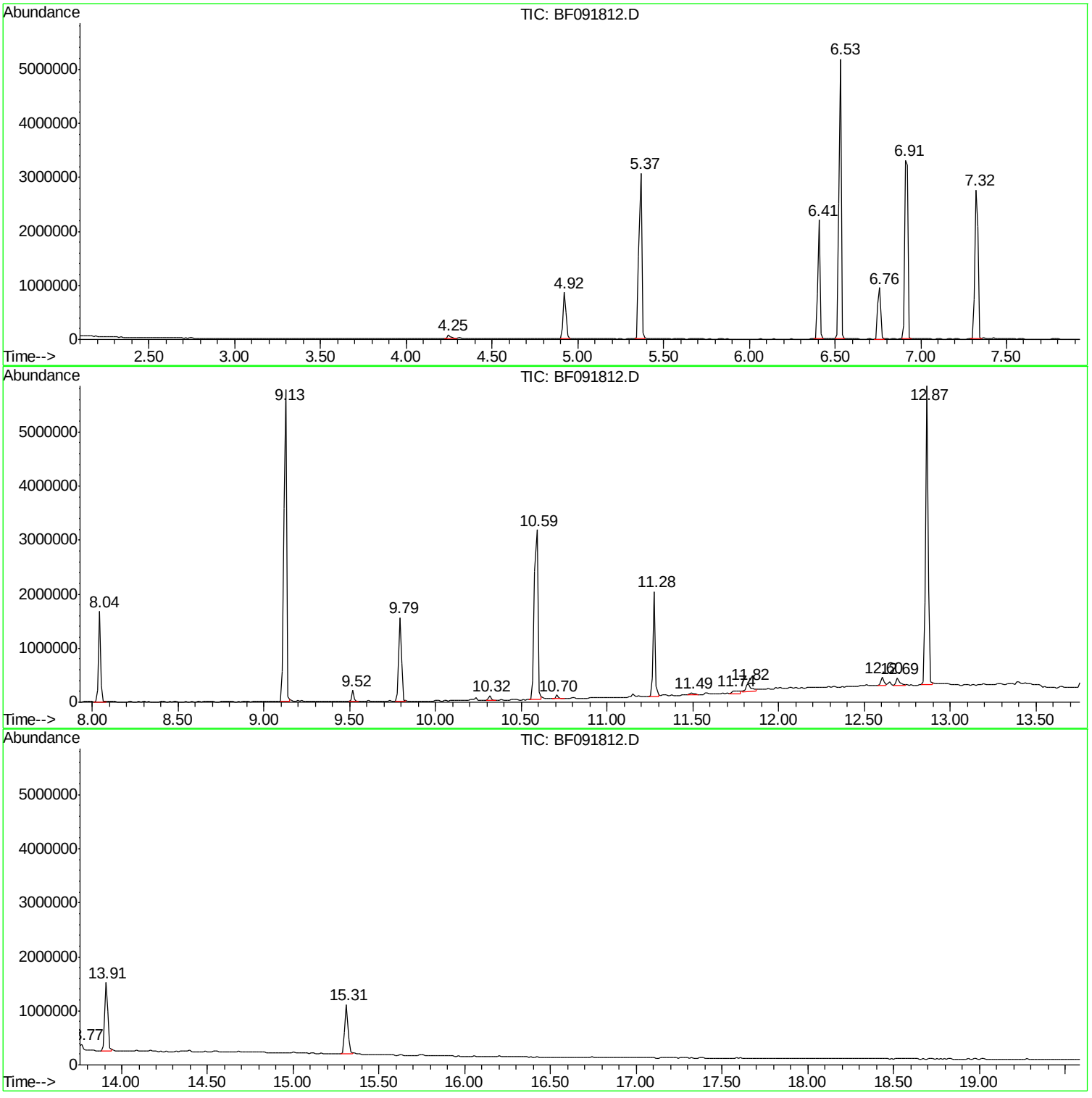
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091812.D
Acq On : 20 Dec 2016 11:36
Operator : UM/SJ
Sample : H6147-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091812.D
Acq On : 20 Dec 2016 11:36
Operator : UM/SJ
Sample : H6147-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

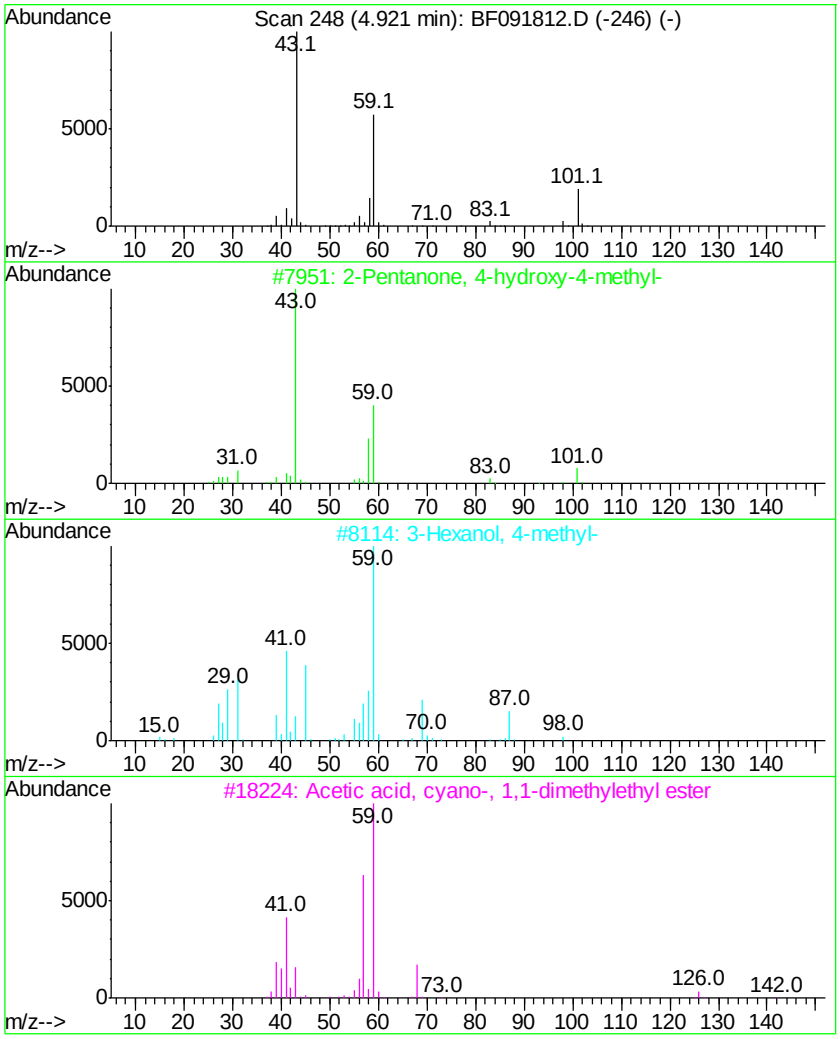
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

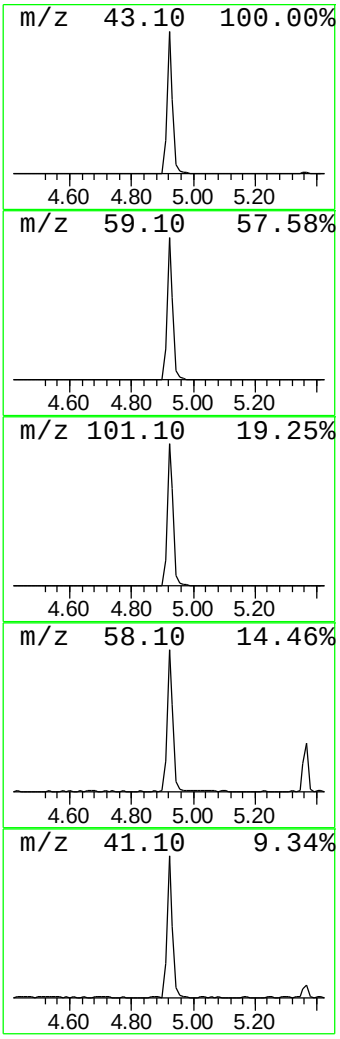
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	19.60 ng	1100050	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Operator : UM/SJ
Sample : H6147-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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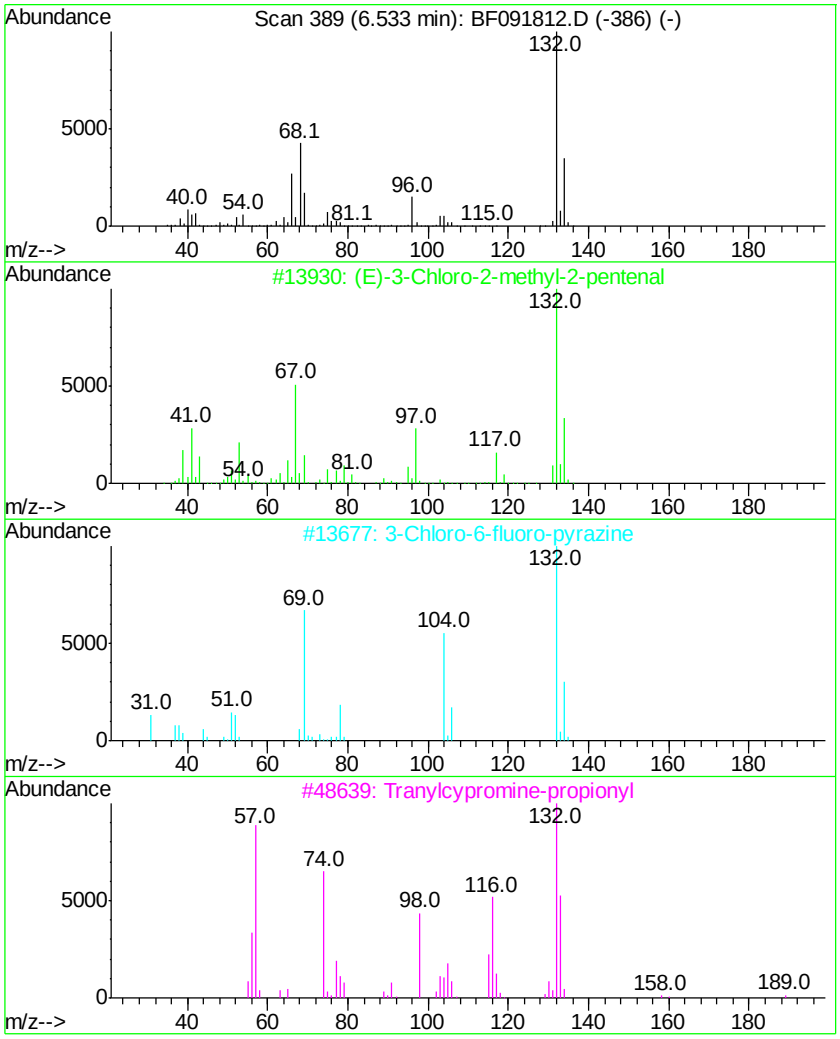
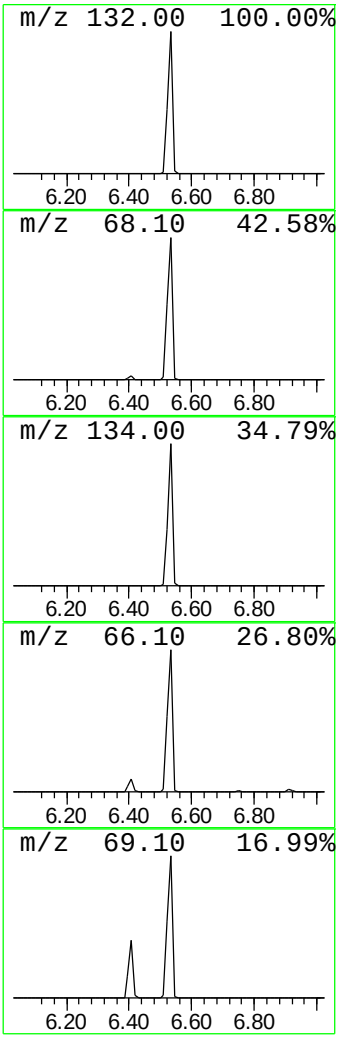
Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	96.07 ng	5390900	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091812.D
Acq On : 20 Dec 2016 11:36
Operator : UM/SJ
Sample : H6147-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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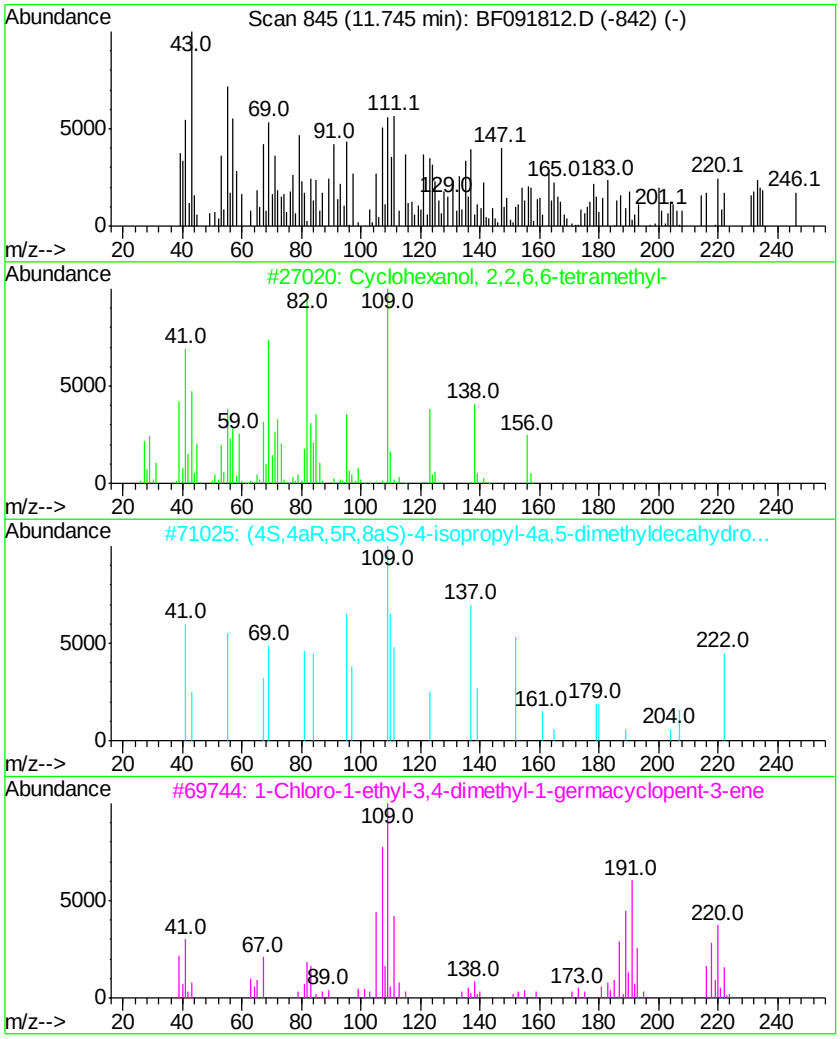
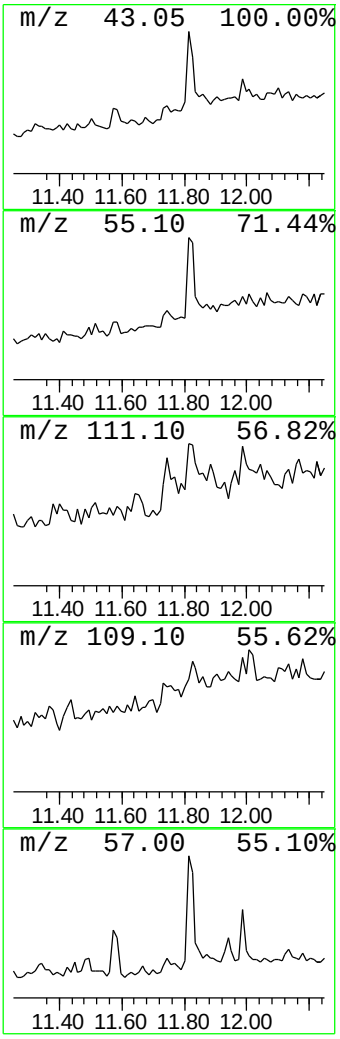
Peak Number 4 unknown11.75 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.01 ng	171441	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 2,2,6,6-tetramethyl-	156	C10H20O	006948-41-0	44
2	(4S,4aR,5R,8aS)-4-isopropyl-4a,5...	222	C15H26O	055897-99-9	30
3	1-Chloro-1-ethyl-3,4-dimethyl-1-...	220	C8H15ClGe	026311-78-4	25
4	1(2H)-Naphthalenone, 3,4,4a,5,6,...	220	C15H24O	056772-20-4	25
5	2,2,6-Trimethyl-1-(3-methylbuta-...	222	C14H22O2	1000191-85-4	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091812.D
Acq On : 20 Dec 2016 11:36
Operator : UM/SJ
Sample : H6147-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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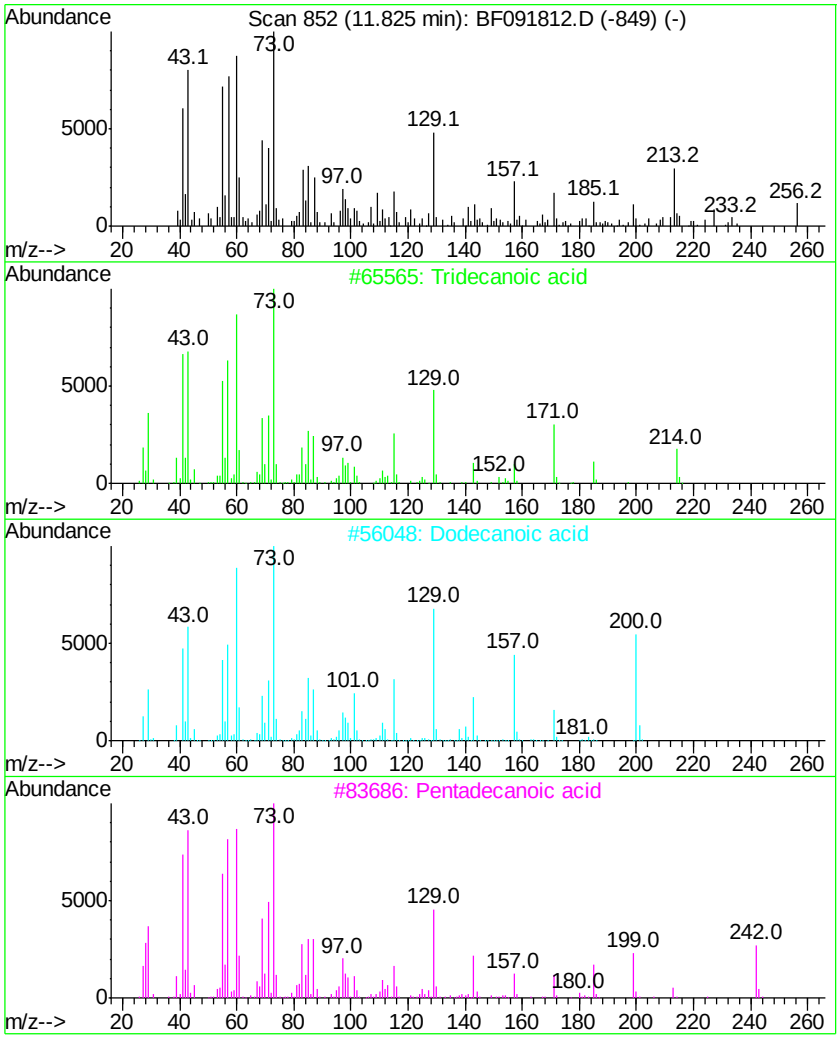
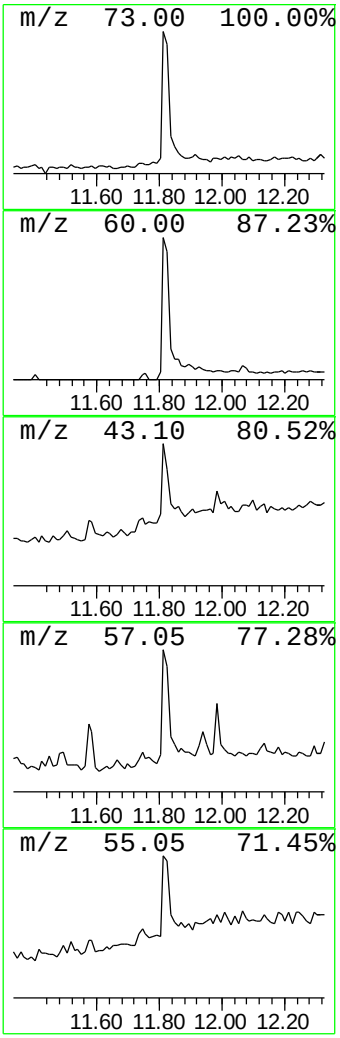
Peak Number 5 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	3.50 ng	298190	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	Dodecanoic acid	200	C12H24O2	000143-07-7	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
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Acq On : 20 Dec 2016 11:36
Operator : UM/SJ
Sample : H6147-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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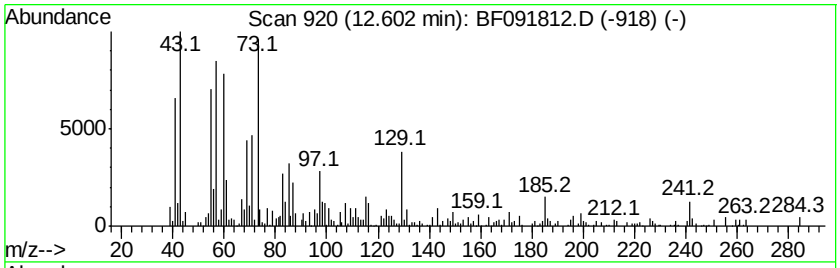
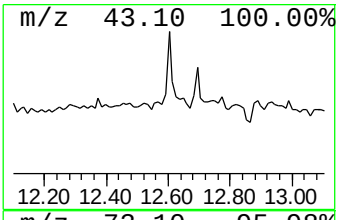
****

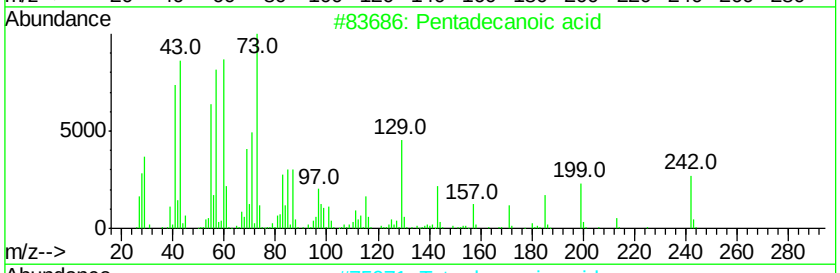
Peak Number 6 Pentadecanoic acid Concentration Rank 5

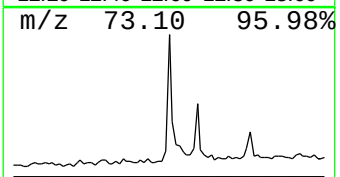
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	2.72 ng	199291	Chrysene-d12	13.91

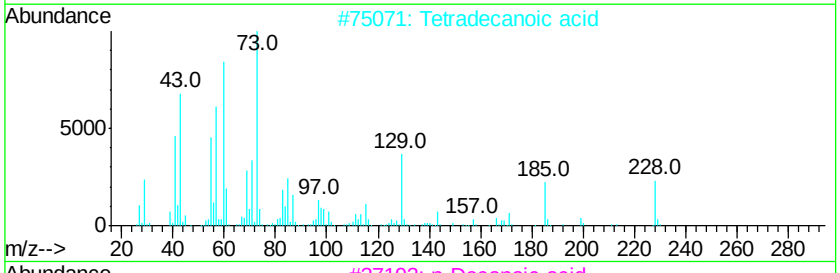
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	n-Decanoic acid	172	C10H20O2	000334-48-5	74
4	Hexadecane	226	C16H34	000544-76-3	45
5	Octane, 1-(ethenylthio)-	172	C10H20S	042779-08-8	38

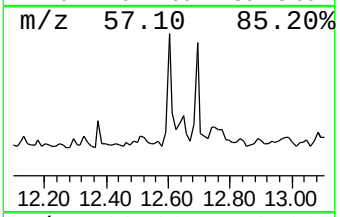


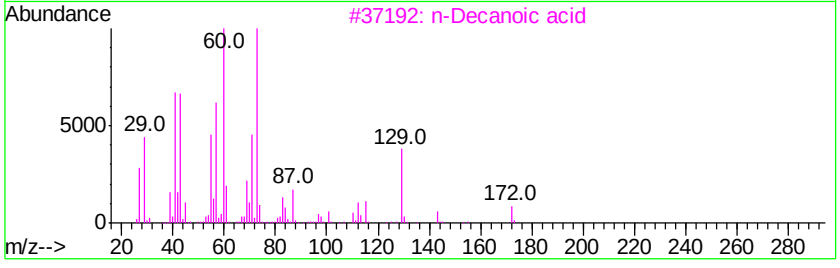


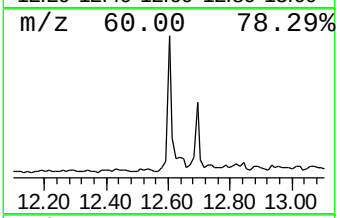


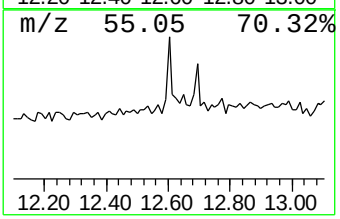












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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

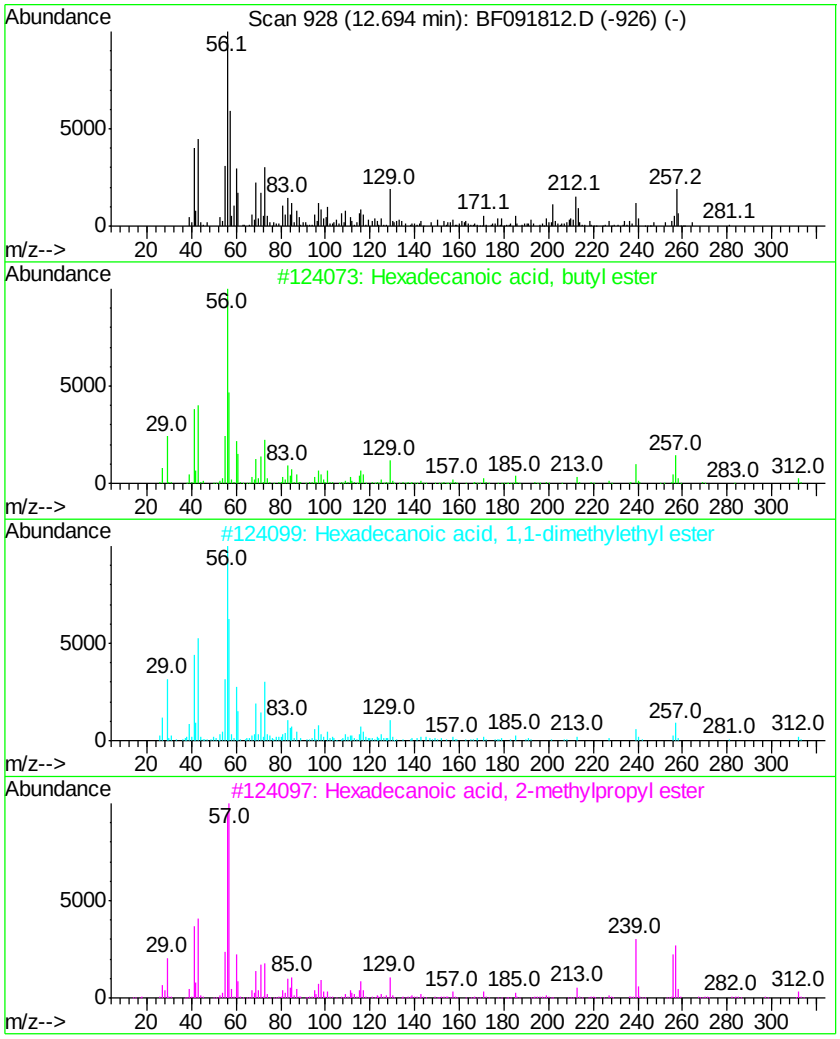
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

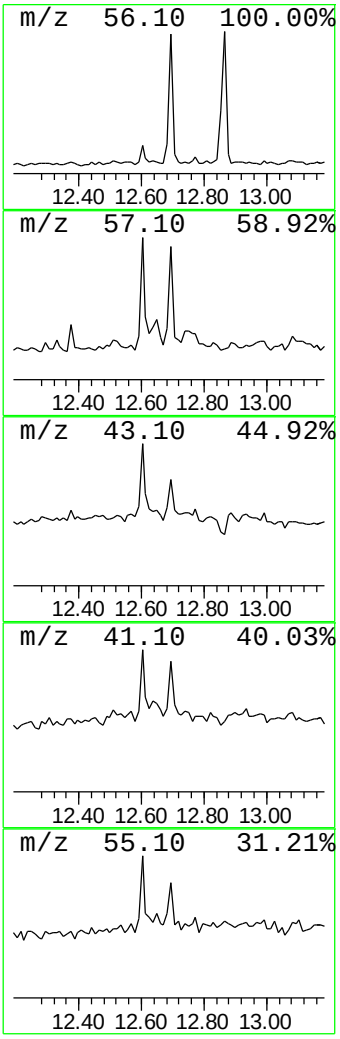
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	2.40 ng	175890	Chrysene-d12	13.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	81
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	68
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
4	Myristic acid isobutyl ester	284	C18H36O2	025263-97-2	47
5	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	43





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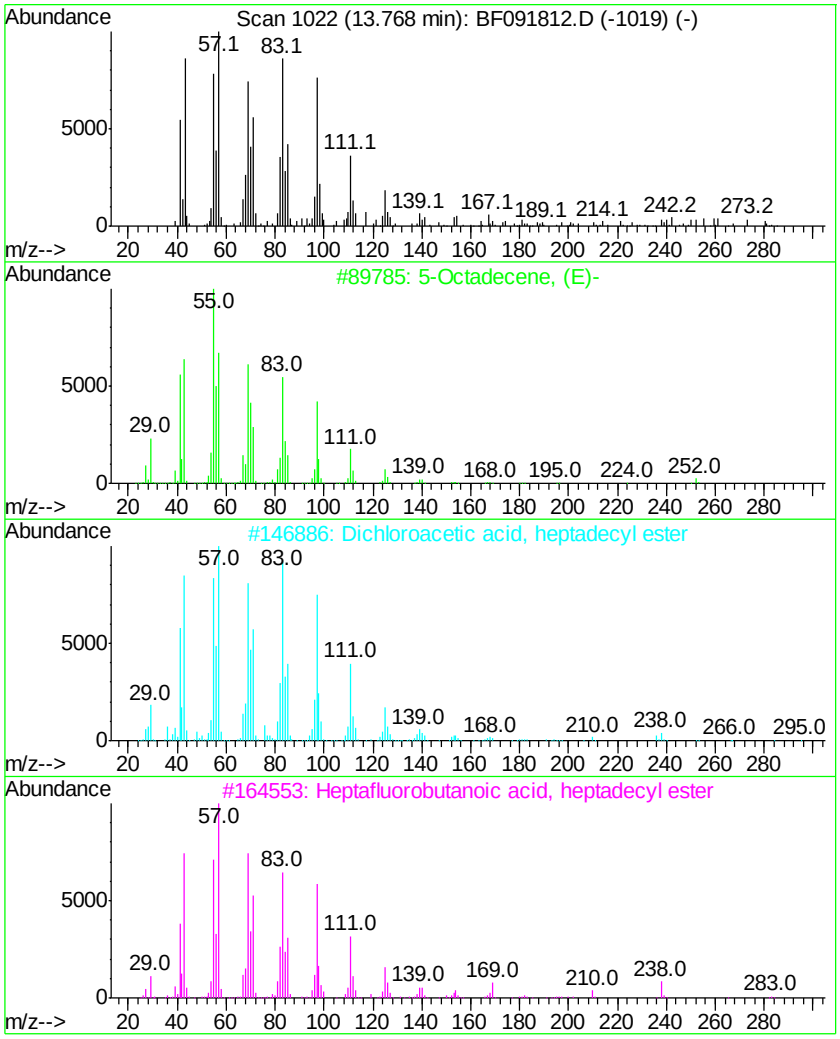
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

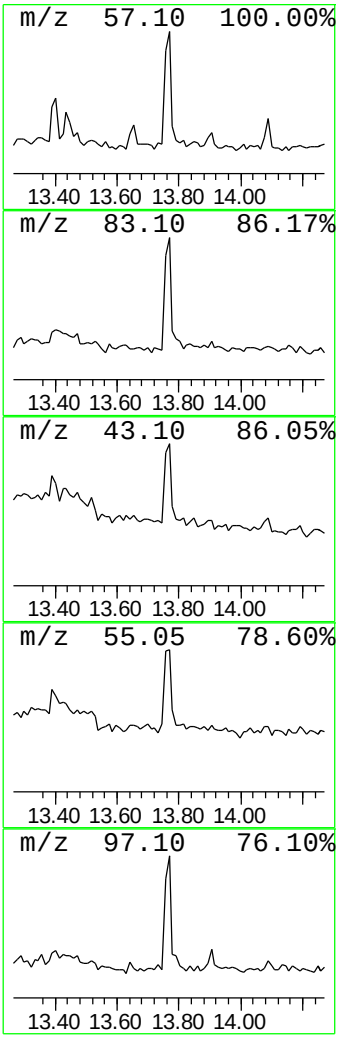
****

Peak Number 8 5-Octadecene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.30 ng	168421	Chrysene-d12	13.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
4	1-Nonadecanol	284	C19H40O	001454-84-8	93
5	1-Octadecanol	270	C18H38O	000112-92-5	93





Tentatively Identified Compound (LSC) summary

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Data File : BF091812.D
Acq On : 20 Dec 2016 11:36
Operator : UM/SJ
Sample : H6147-04
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	19.6	ng	1100050	1	6.76	1122230	20.0
unknown6.53	6.53	96.1	ng	5390900	1	6.76	1122230	20.0
unknown11.75	11.75	2.0	ng	171441	4	11.28	1701930	20.0
Tridecanoic acid	11.83	3.5	ng	298190	4	11.28	1701930	20.0
Pentadecanoic acid	12.60	2.7	ng	199291	5	13.91	1465050	20.0
Hexadecanoic acid...	12.69	2.4	ng	175890	5	13.91	1465050	20.0
5-Octadecene, (E)-	13.77	2.3	ng	168421	5	13.91	1465050	20.0