LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100976.D
Acq On : 29 Nov 2017 14:28
Operator : SJ/JU
Sample : I6616-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

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-BF110817.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	5.081	505	509	520	rVB	82796	108301	5.80%	0.655%
2	5.469	570	575	578	rBV	1440518	1487102	79.57%	8.996%
3	6.487	742	748	754	rVB	1480033	1575807	84.32%	9.533%
4	6.622	766	771	774	rBV	1756794	1623434	86.87%	9.821%
5	6.851	806	810	813	rBV	537368	436578	23.36%	2.641%
6	7.010	832	837	840	rBV	1404854	1263263	67.60%	7.642%
7	7.416	901	906	909	rBV	1053297	1005550	53.81%	6.083%
8	8.133	1024	1028	1031	rVB	750635	590452	31.59%	3.572%
9	8.716	1124	1127	1131	rVB	32168	24459	1.31%	0.148%
10	9.210	1206	1211	1214	rBV	2204165	1868846	100.00%	11.306%
11	9.280	1220	1223	1226	rBV	54822	43539	2.33%	0.263%
12	9.598	1274	1277	1280	rBV	143865	120715	6.46%	0.730%
13	9.810	1308	1313	1317	rVB	71133	55653	2.98%	0.337%
14	9.886	1322	1326	1330	rVB	795578	670766	35.89%	4.058%
15	10.080	1355	1359	1365	rVB5	29026	36620	1.96%	0.222%
16	10.310	1395	1398	1401	rVB	74869	56482	3.02%	0.342%
17	10.527	1431	1435	1438	rBV	29904	33388	1.79%	0.202%
18	10.598	1444	1447	1453	rVB	56090	53386	2.86%	0.323%
19	10.680	1457	1461	1464	rVV	1188398	1094184	58.55%	6.619%
20	10.780	1475	1478	1483	rBV2	68365	102363	5.48%	0.619%
21	10.980	1508	1512	1515	rBV3	17755	25692	1.37%	0.155%
22	11.227	1551	1554	1557	rBV	48293	38786	2.08%	0.235%
23	11.257	1557	1559	1565	rVB3	32139	34783	1.86%	0.210%
24	11.374	1575	1579	1582	rBV	753193	619174	33.13%	3.746%
25	11.657	1624	1627	1630	rBV	38697	29580	1.58%	0.179%
26	11.898	1662	1668	1675	rBV3	185251	191532	10.25%	1.159%
27	12.063	1693	1696	1699	rBV	42885	35433	1.90%	0.214%
28	12.410	1753	1755	1759	rBV4	23676	28265	1.51%	0.171%
29	12.451	1759	1762	1766	rVV3	34524	38213	2.04%	0.231%
30	12.586	1782	1785	1792	rBV	126824	133847	7.16%	0.810%
31	12.680	1797	1801	1806	rBV	134083	134762	7.21%	0.815%
32	12.816	1819	1824	1827	rBV2	104384	120823	6.47%	0.731%
33	12.957	1844	1848	1852	rBV	1391043	1249581	66.86%	7.559%
34	13.157	1877	1882	1884	rBV4	14302	27039	1.45%	0.164%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I6616-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.398	1921	1923	1926	rBV	26555	21630	1.16%	0.131%
36	13.521	1940	1944	1947	rBV3	23808	34247	1.83%	0.207%
37	13.845	1996	1999	2005	rVB3	82372	96980	5.19%	0.587%
38	13.986	2019	2023	2024	rBV	67964	66393	3.55%	0.402%
39	14.015	2024	2028	2031	rVV	487119	490502	26.25%	2.967%
40	14.039	2031	2032	2038	rVB	58374	42448	2.27%	0.257%
41	15.051	2201	2204	2208	rBV	64443	97189	5.20%	0.588%
42	15.139	2217	2219	2226	rVB5	41539	59063	3.16%	0.357%
43	15.421	2264	2267	2272	rVB	46414	60978	3.26%	0.369%
44	15.486	2273	2278	2285	rVB	363158	451967	24.18%	2.734%
45	15.927	2349	2353	2358	rVB	47803	66370	3.55%	0.402%
46	16.427	2435	2438	2444	rVB4	30242	49984	2.67%	0.302%
47	16.951	2525	2527	2532	rVB2	27406	34087	1.82%	0.206%

Sum of corrected areas: 16530236

LSC Report - Integrated Chromatogram

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Operator : SJ/JU
Sample : I6616-01
Misc :
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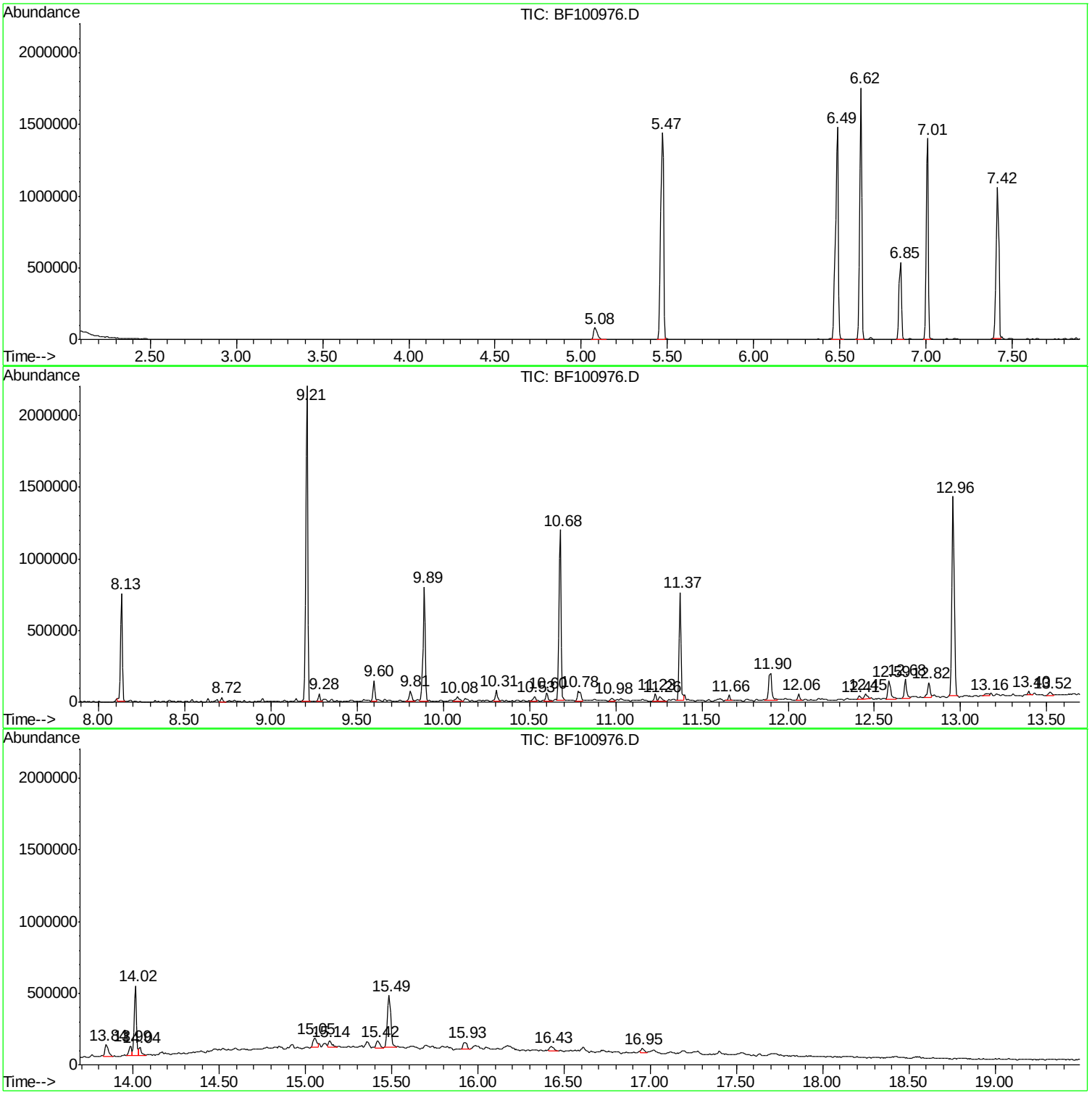
Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF100976.D
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Operator : SJ/JU
Sample : I6616-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

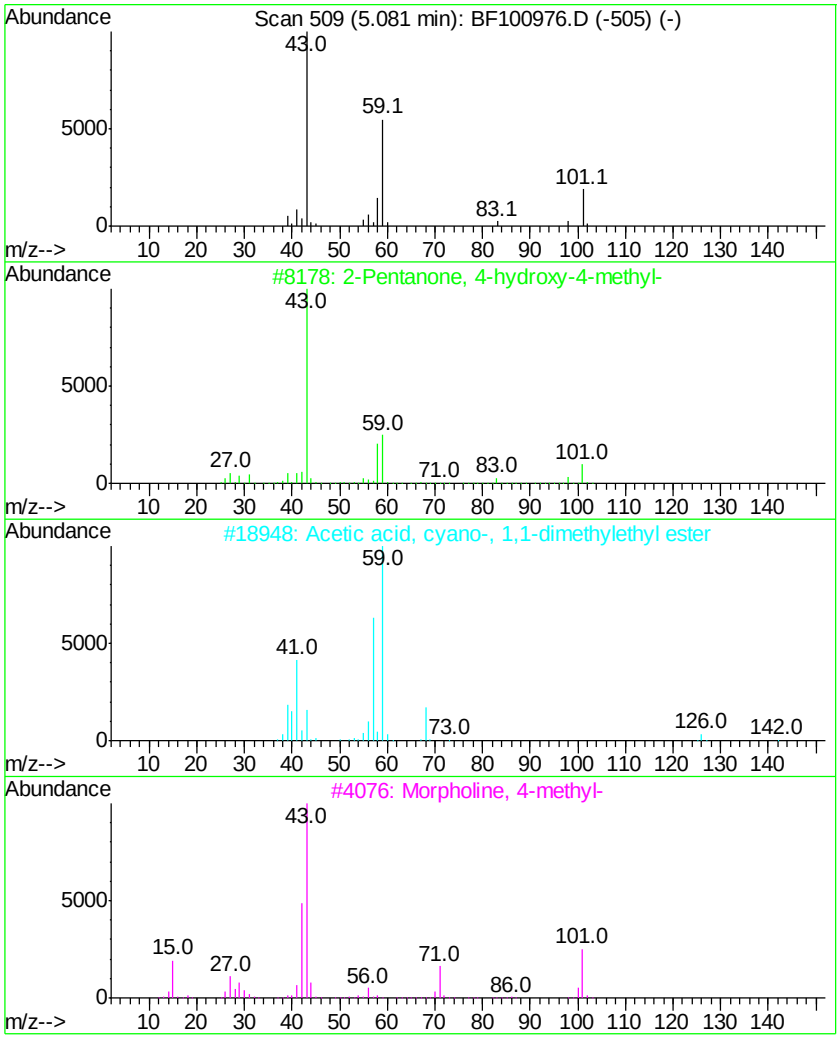
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

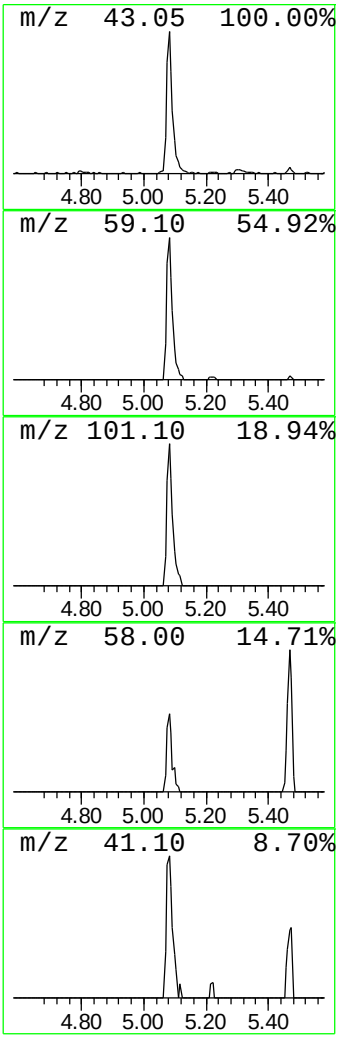
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	4.96 ng	108301	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Misc :
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Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

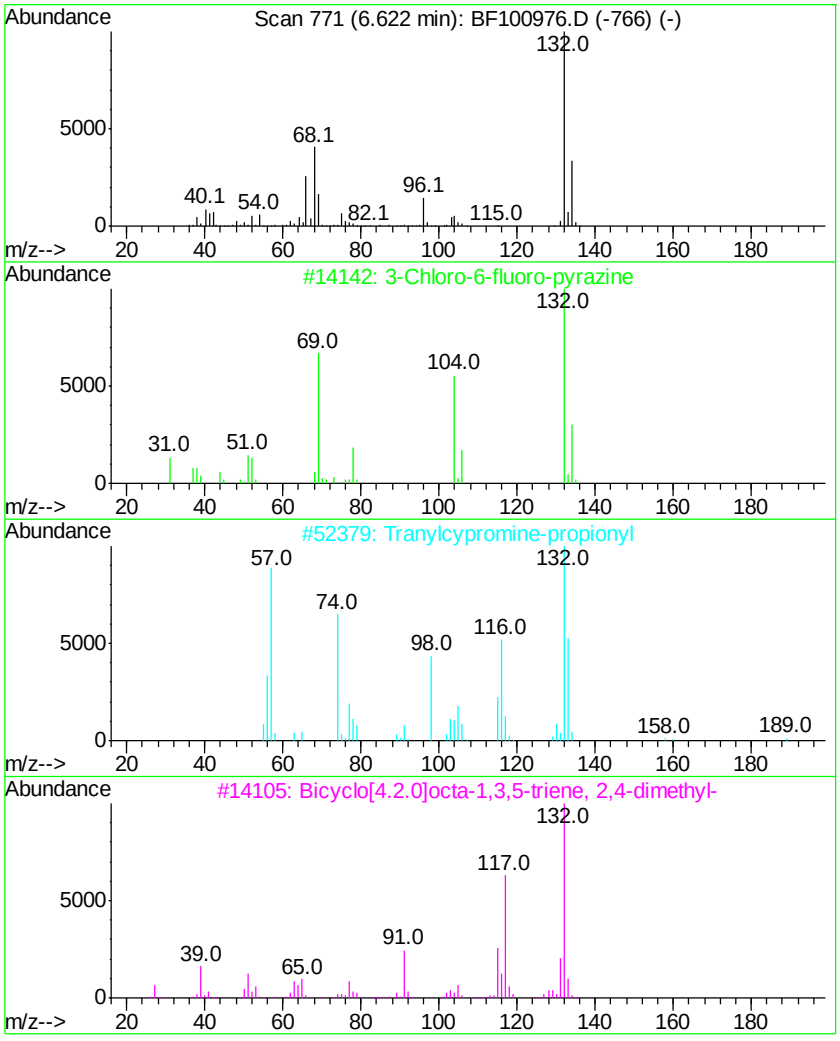
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

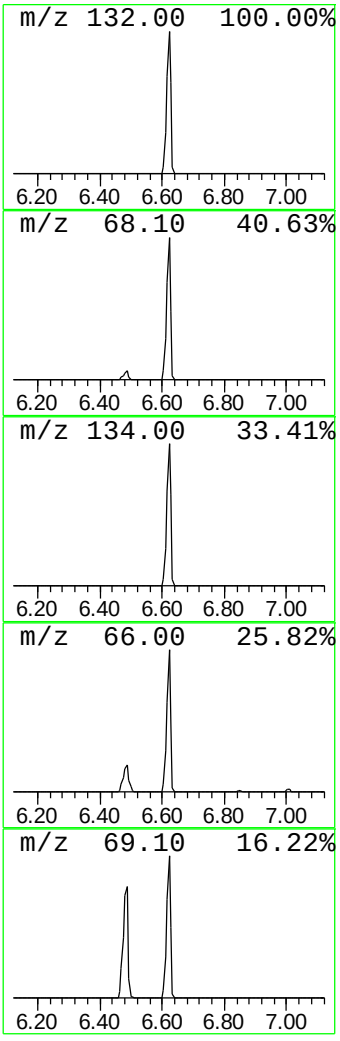
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	74.37 ng	1623430	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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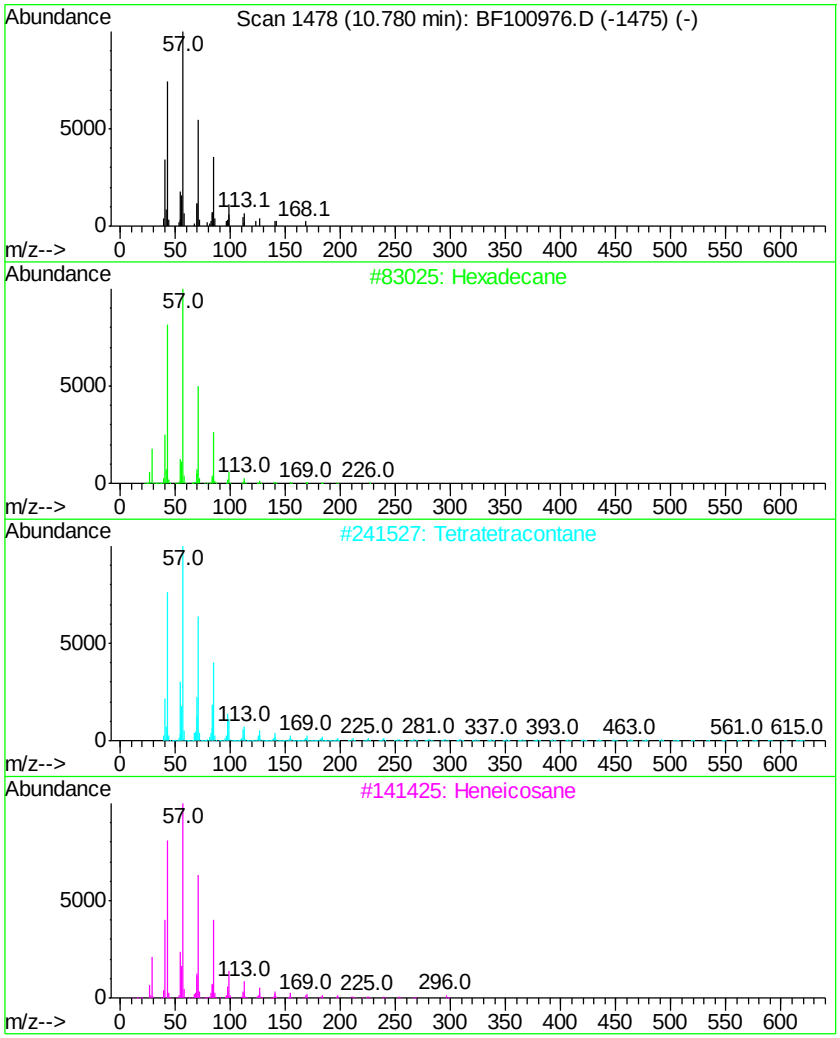
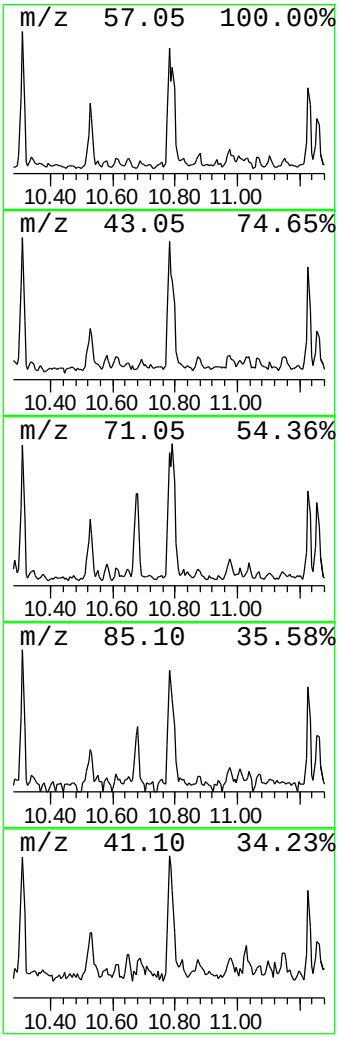
Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	3.31 ng	102363	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Heneicosane	296	C21H44	000629-94-7	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Tetracosane	338	C24H50	000646-31-1	86





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Data File : BF100976.D
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Operator : SJ/JU
Sample : I6616-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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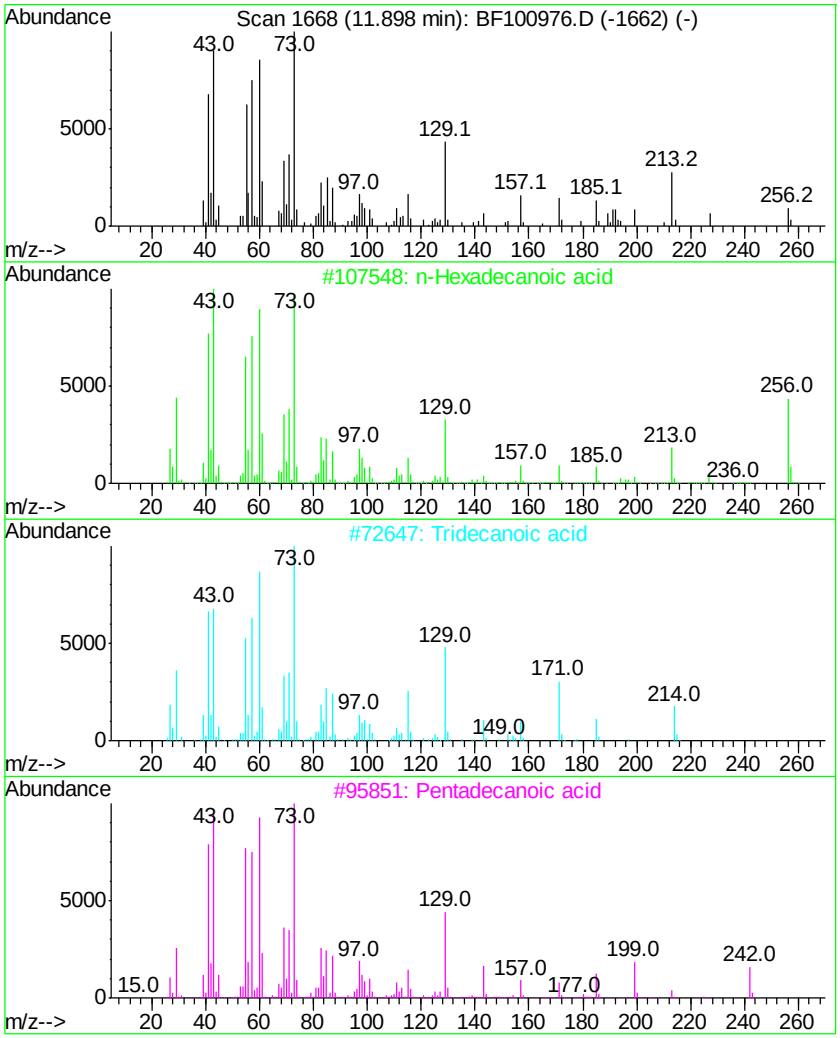
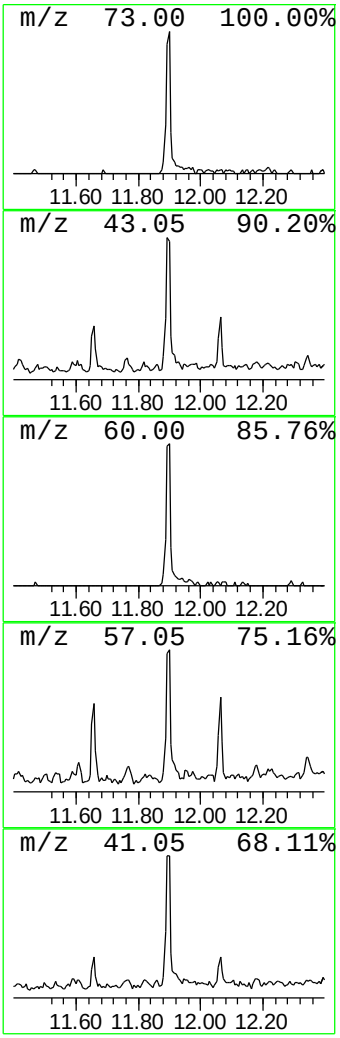
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	6.19 ng	191532	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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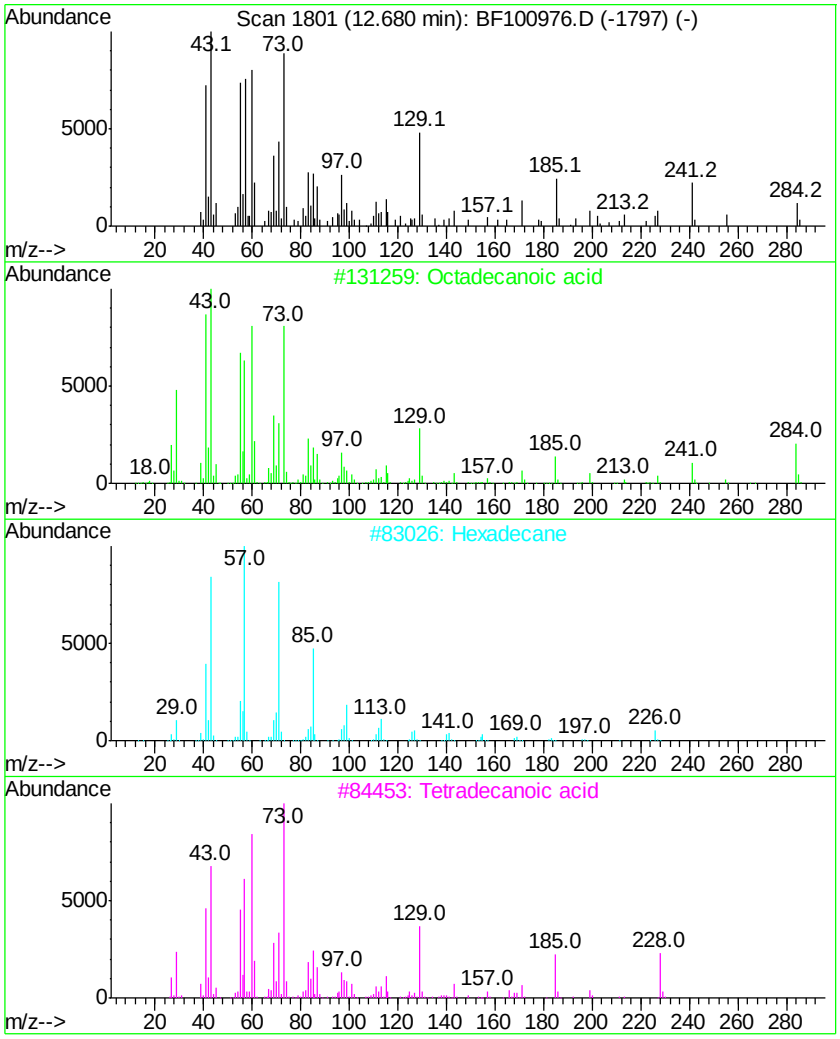
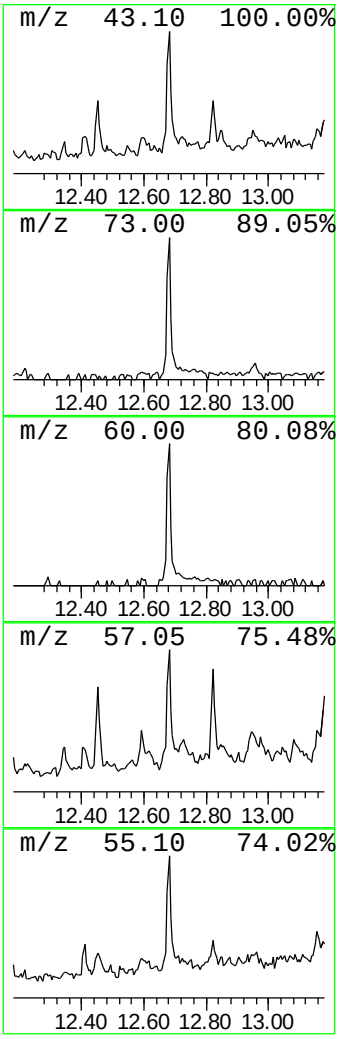
Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	4.35 ng	134762	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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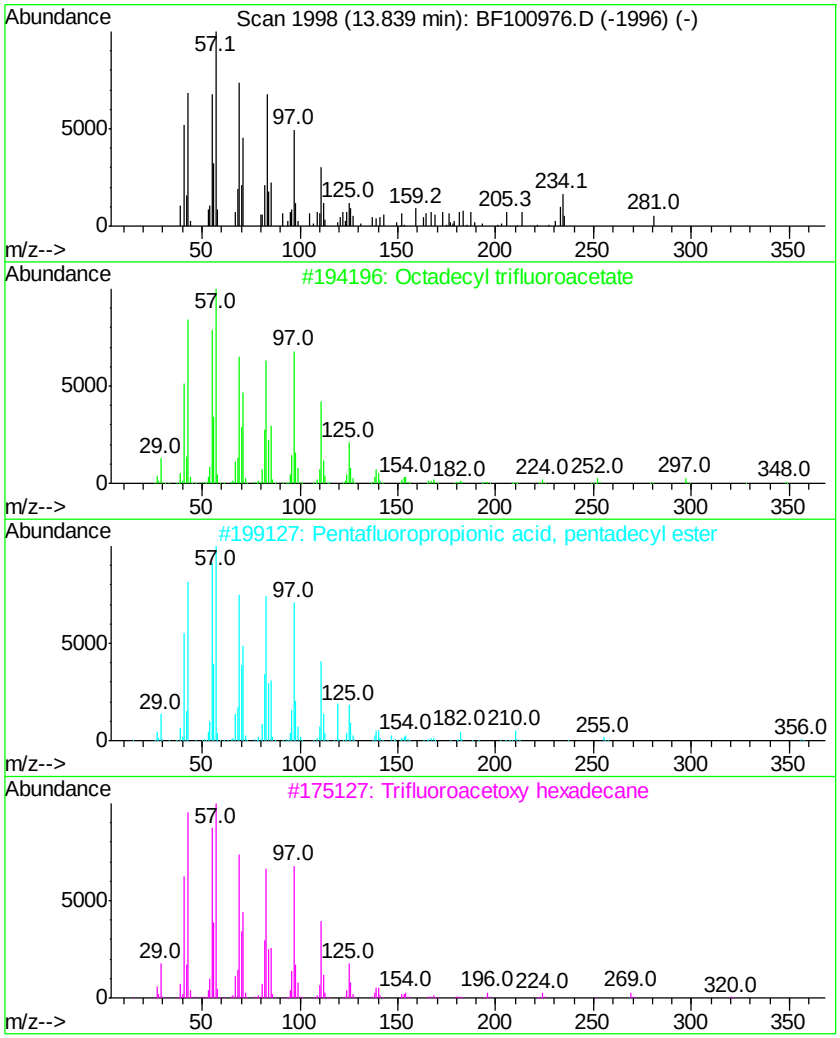
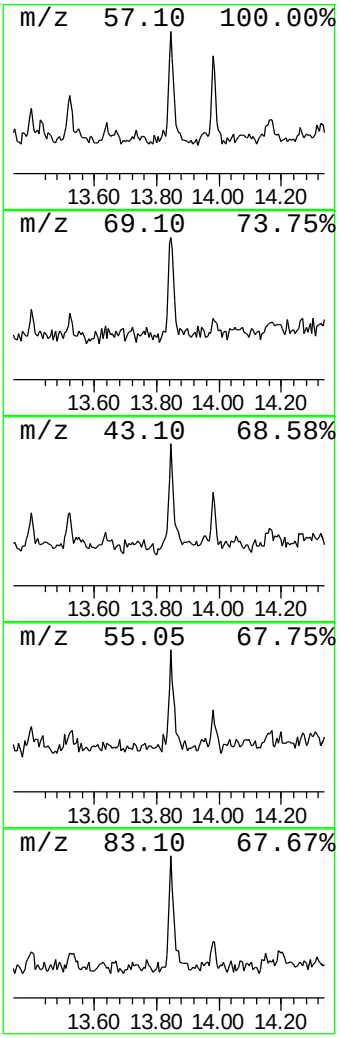
Peak Number 7 Octadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.95 ng	96980	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	83
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	81
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	74





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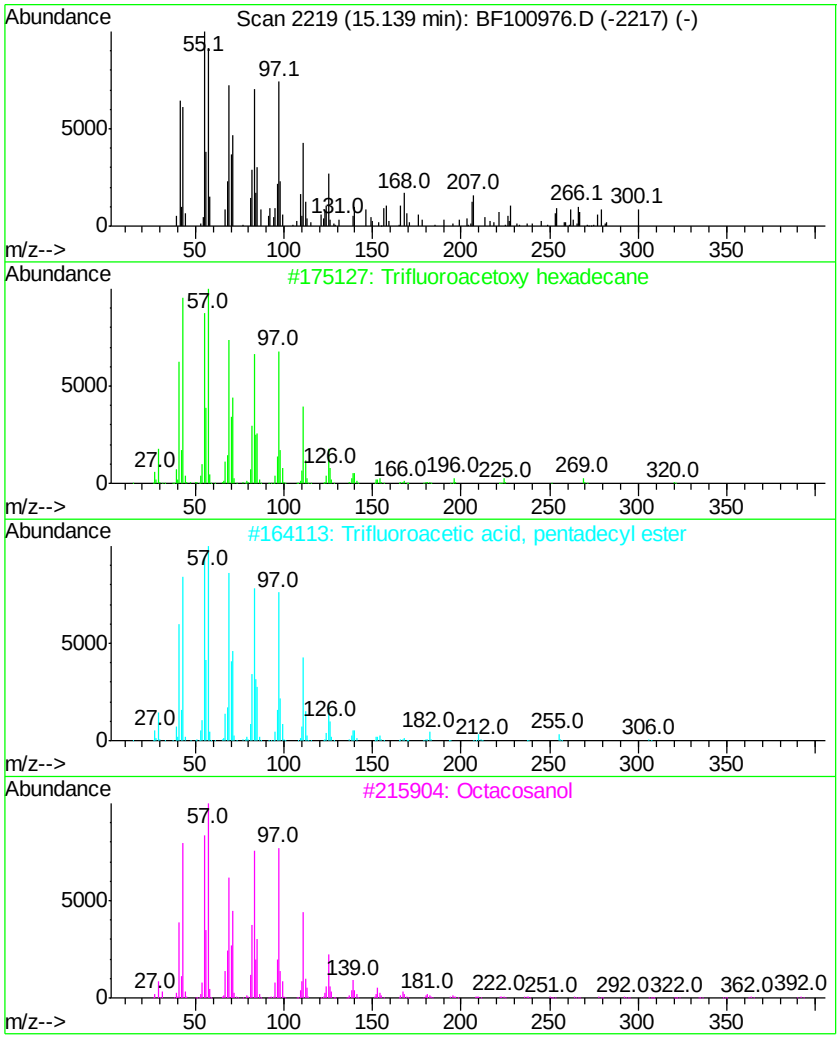
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

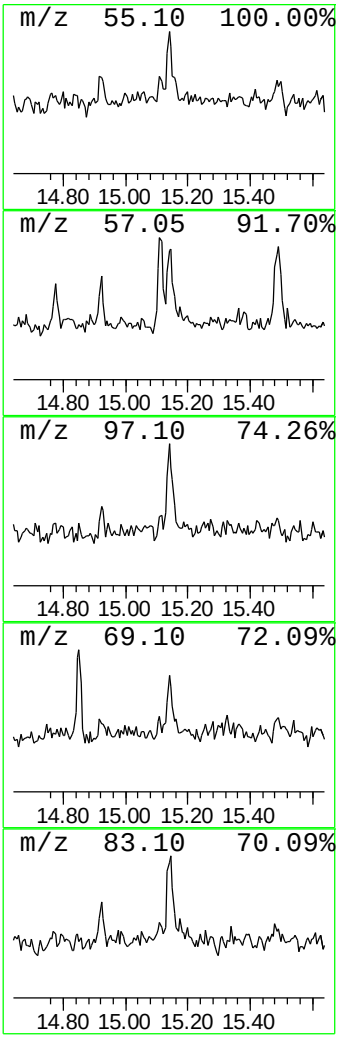
****

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	2.61 ng	59063	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	76
3	Octacosanol	410	C28H58O	000557-61-9	72
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	68
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	68





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Data File : BF100976.D
Acq On : 29 Nov 2017 14:28
Operator : SJ/JU
Sample : I6616-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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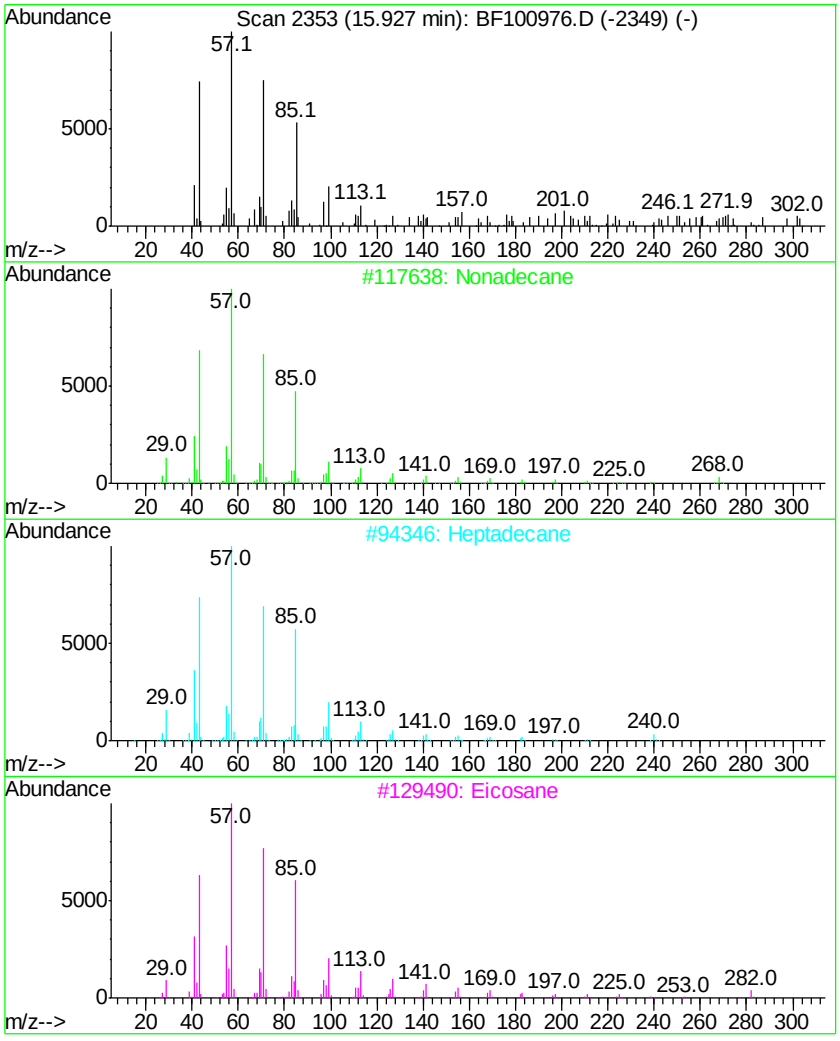
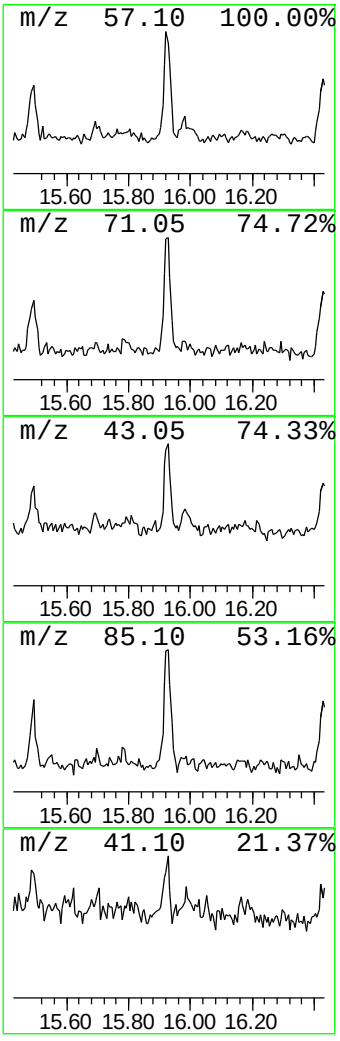
Peak Number 9 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.94 ng	66370	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Heptadecane	240	C17H36	000629-78-7	90
3	Eicosane	282	C20H42	000112-95-8	81
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	81
5	Pentadecane	212	C15H32	000629-62-9	76





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Sample : I6616-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

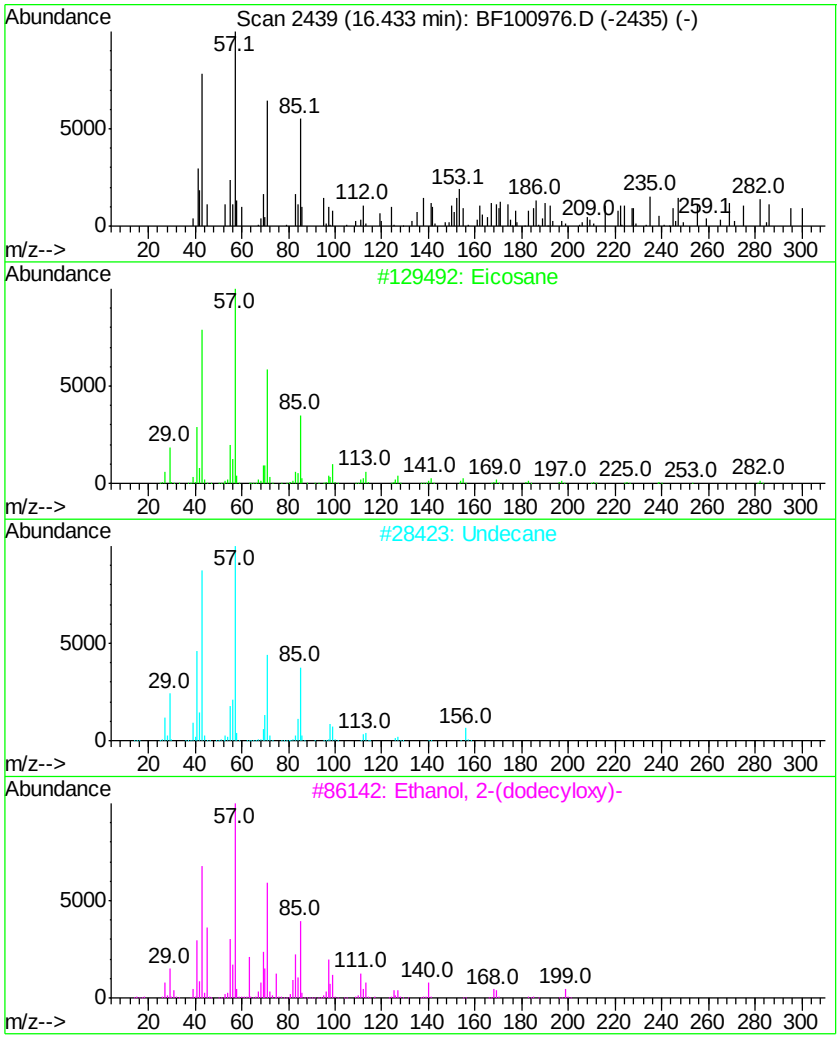
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

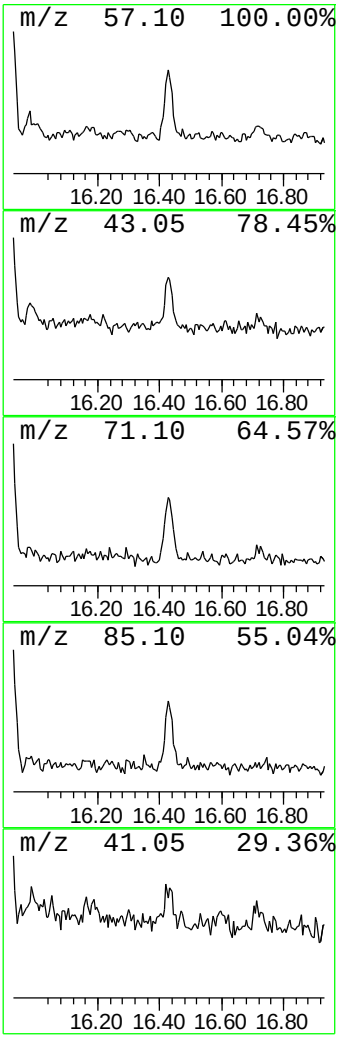
****

Peak Number 10 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	2.21 ng	49984	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	55
2	Undecane	156	C11H24	001120-21-4	49
3	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	43
4	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	38
5	Tetradecane	198	C14H30	000629-59-4	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112917\
Data File : BF100976.D
Acq On : 29 Nov 2017 14:28
Operator : SJ/JU
Sample : I6616-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-LOT-SP1-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	5.0	ng	108301	1	6.85	436578	20.0
unknown6.62	6.62	74.4	ng	1623430	1	6.85	436578	20.0
Hexadecane	10.78	3.3	ng	102363	4	11.37	619174	20.0
n-Hexadecanoic acid	11.90	6.2	ng	191532	4	11.37	619174	20.0
Octadecanoic acid	12.68	4.3	ng	134762	4	11.37	619174	20.0
Octadecyl trifluo...	13.84	4.0	ng	96980	5	14.02	490502	20.0
Trifluoroacetoxy ...	15.14	2.6	ng	59063	6	15.49	451967	20.0
Nonadecane	15.93	2.9	ng	66370	6	15.49	451967	20.0
Eicosane	16.43	2.2	ng	49984	6	15.49	451967	20.0