LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116842.D
Acq On : 5 Sep 2019 17:08
Operator : HP/JU
Sample : K4694-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-1-4-(0-1.5)

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-BF083019.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	5.457	569	573	586	rBV	666836	637074	73.85%	5.366%
2	6.475	742	746	756	rBV	859660	731158	84.76%	6.159%
3	6.616	766	770	773	rBV	880173	725782	84.13%	6.114%
4	6.845	805	809	818	rBV	694274	552271	64.02%	4.652%
5	7.004	832	836	839	rBV	631122	543202	62.97%	4.576%
6	7.398	896	903	910	rBV	460039	436269	50.57%	3.675%
7	8.128	1023	1027	1039	rBV	934407	759339	88.02%	6.396%
8	8.839	1145	1148	1152	rBV	25986	21012	2.44%	0.177%
9	8.886	1152	1156	1163	rVV	23958	34641	4.02%	0.292%
10	9.198	1205	1209	1212	rBV	1105275	858942	99.57%	7.235%
11	9.586	1273	1275	1280	rBV	74242	61798	7.16%	0.521%
12	9.880	1321	1325	1329	rBV	1077103	862652	100.00%	7.266%
13	10.080	1353	1359	1362	rBV3	12096	13065	1.51%	0.110%
14	10.663	1455	1458	1462	rBV	520354	444379	51.51%	3.743%
15	10.786	1476	1479	1487	rBV5	12401	21401	2.48%	0.180%
16	10.880	1491	1495	1497	rVV3	12598	14164	1.64%	0.119%
17	10.910	1497	1500	1503	rVB3	13110	11638	1.35%	0.098%
18	11.027	1516	1520	1524	rBV4	13358	14611	1.69%	0.123%
19	11.063	1524	1526	1529	rBV	14095	11971	1.39%	0.101%
20	11.139	1535	1539	1541	rVB	10446	10563	1.22%	0.089%
21	11.169	1541	1544	1549	rBV4	11294	14265	1.65%	0.120%
22	11.221	1550	1553	1558	rBV5	21971	26340	3.05%	0.222%
23	11.363	1573	1577	1579	rBV	935102	778299	90.22%	6.556%
24	11.386	1579	1581	1584	rVV	169663	131639	15.26%	1.109%
25	11.439	1587	1590	1593	rVB	34955	34562	4.01%	0.291%
26	11.521	1601	1604	1605	rBV	13790	12387	1.44%	0.104%
27	11.592	1612	1616	1619	rBV2	28988	37158	4.31%	0.313%
28	11.657	1625	1627	1630	rBV2	15037	14505	1.68%	0.122%
29	11.757	1642	1644	1647	rBV3	16288	15401	1.79%	0.130%
30	11.863	1660	1662	1663	rBV2	19216	14142	1.64%	0.119%
31	11.886	1663	1666	1669	rVV2	169735	149174	17.29%	1.257%
32	11.974	1679	1681	1684	rBV	30344	23420	2.71%	0.197%
33	12.157	1710	1712	1714	rBV2	19814	15048	1.74%	0.127%
34	12.574	1780	1783	1786	rBV	277433	225972	26.20%	1.903%

LSC Area Percent Report

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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-1-4-(0-1.5)

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-BF083019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.668	1797	1799	1802	rBV2	70220	58409	6.77%	0.492%
36	12.804	1819	1822	1828	rVB	228035	218377	25.31%	1.839%
37	12.945	1842	1846	1849	rBV	770243	708583	82.14%	5.969%
38	13.839	1996	1998	2007	rVB3	117502	164835	19.11%	1.388%
39	13.974	2018	2021	2023	rBV	655528	660350	76.55%	5.562%
40	13.998	2023	2025	2028	rVB	730182	646447	74.94%	5.445%
41	14.845	2166	2169	2172	rBV	122325	124891	14.48%	1.052%
42	15.033	2198	2201	2208	rVB	107823	178217	20.66%	1.501%
43	15.104	2210	2213	2216	rVB2	91029	98552	11.42%	0.830%
44	15.392	2260	2262	2265	rVV	52192	51880	6.01%	0.437%
45	15.462	2269	2274	2285	rVB	426882	702876	81.48%	5.921%

Sum of corrected areas: 11871661

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
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Sample : K4694-01 2X
Misc :
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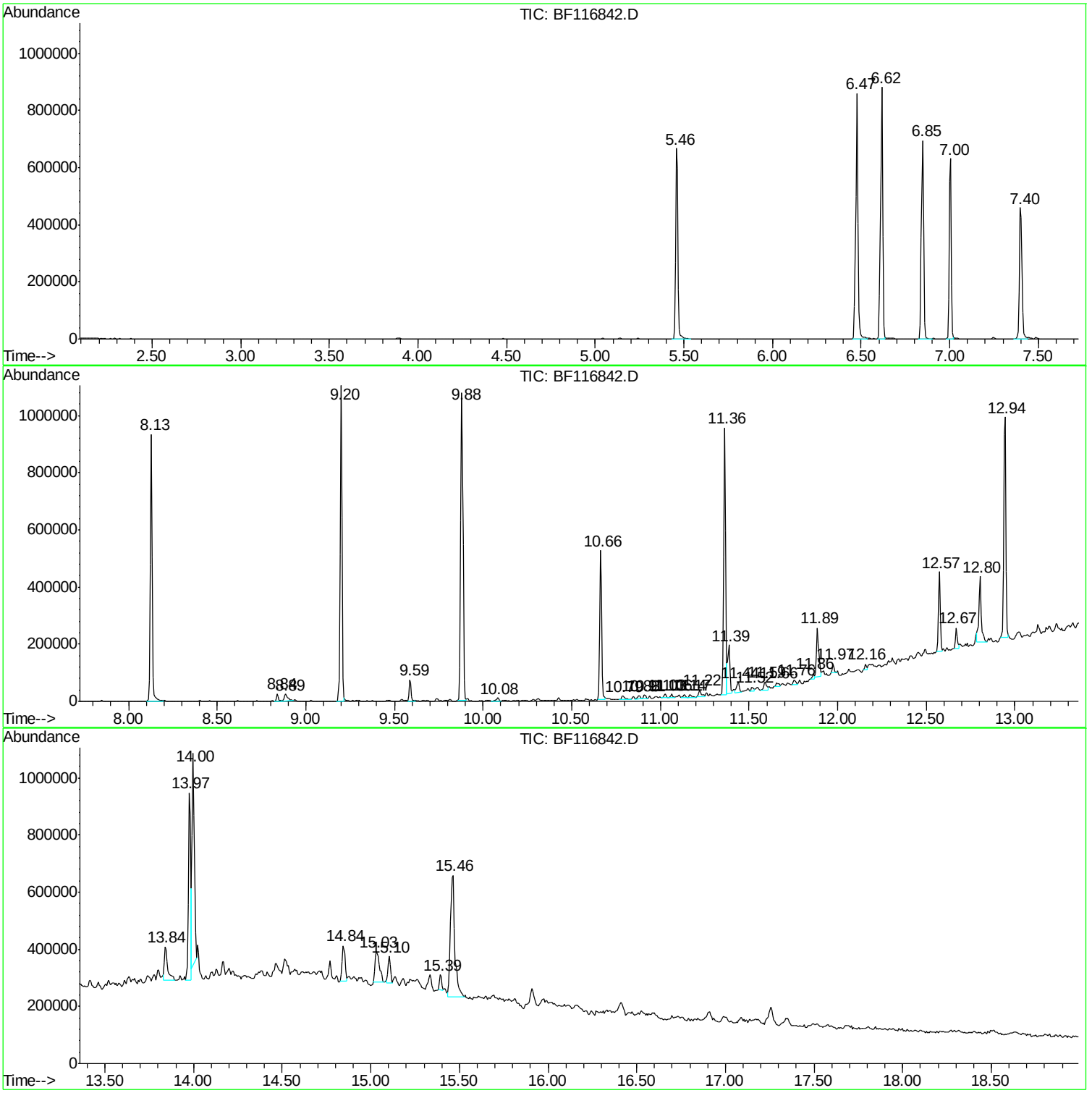
Instrument : BNA_F
ClientSampleId : T1-1-4-(0-1.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116842.D
Acq On : 5 Sep 2019 17:08
Operator : HP/JU
Sample : K4694-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-1-4-(0-1.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

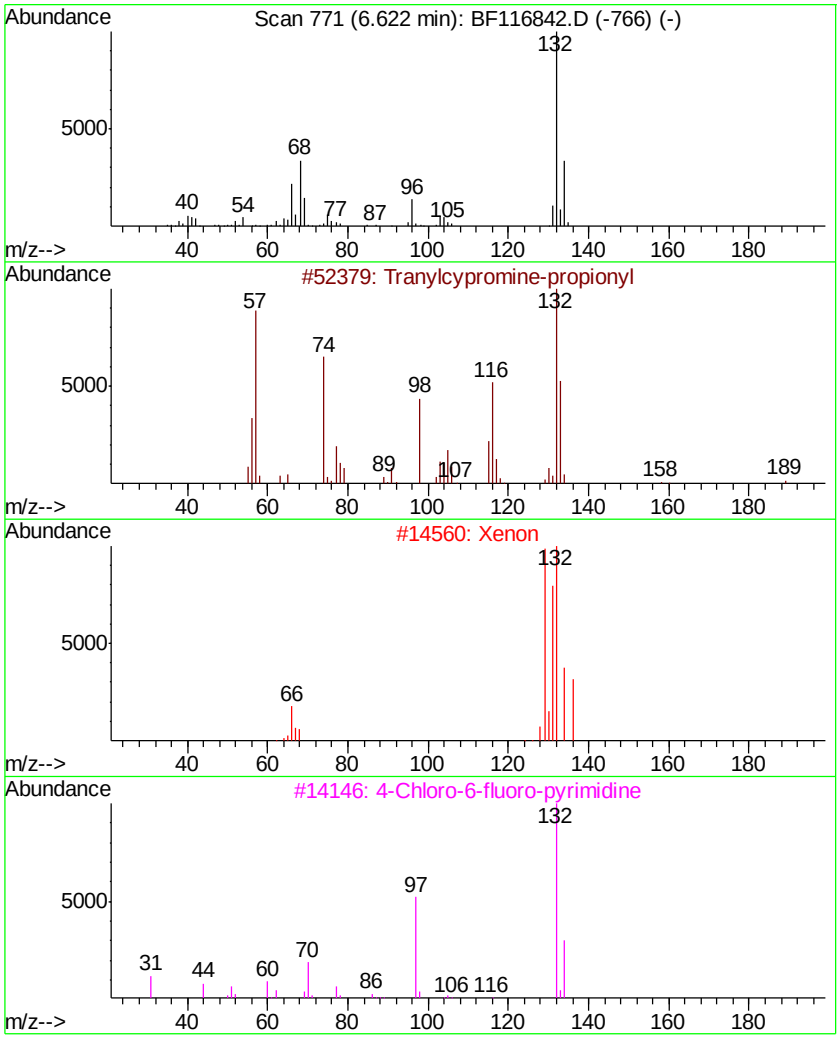
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

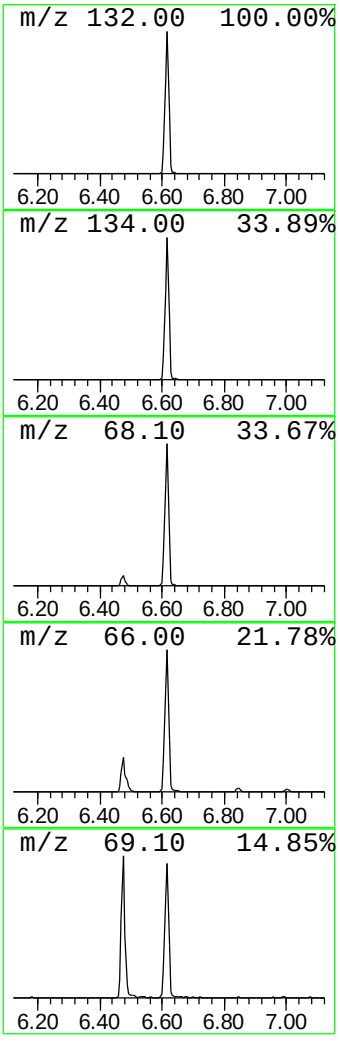
****

Peak Number 1 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	26.28 ng	725782	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	Xenon	132	Xe	007440-63-3	9
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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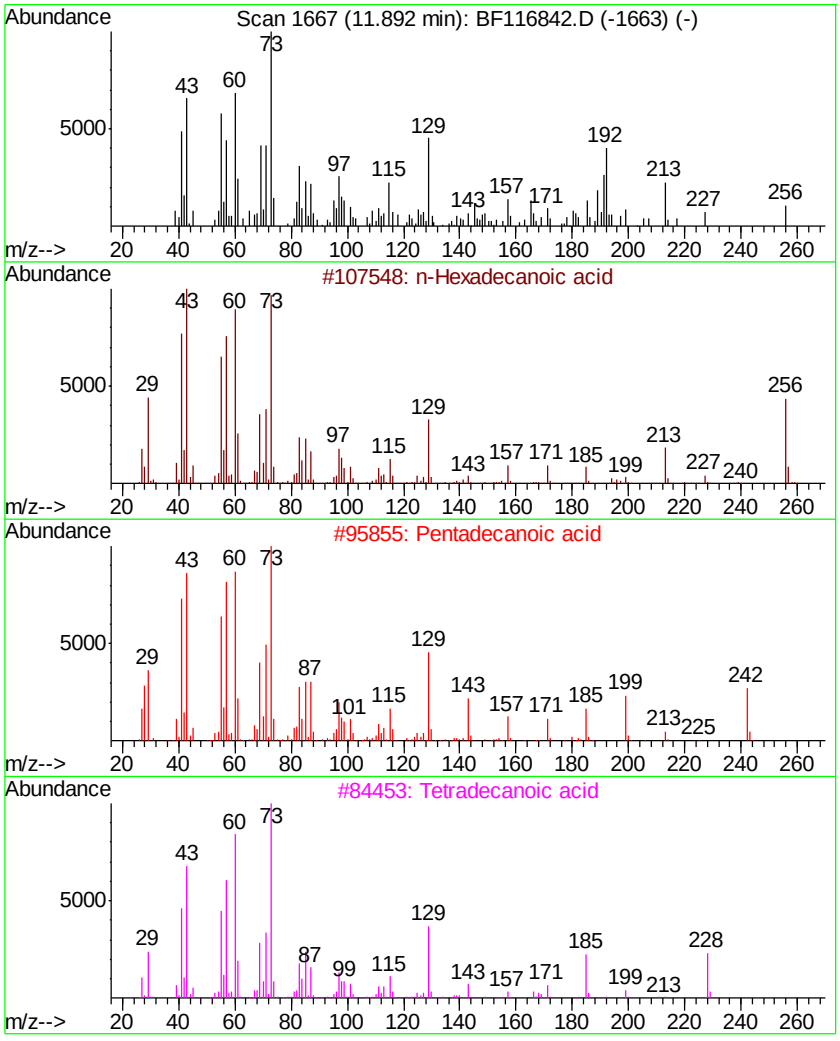
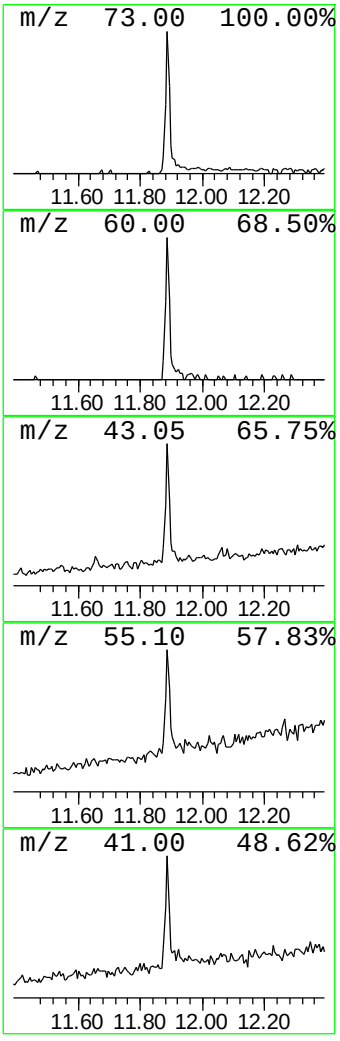
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	3.83 ng	149174	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	50
5	Tridecanoic acid	214	C13H26O2	000638-53-9	46





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Data File : BF116842.D
Acq On : 5 Sep 2019 17:08
Operator : HP/JU
Sample : K4694-01 2X
Misc :
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Instrument : BNA_F
ClientSampleId : T1-1-4-(0-1.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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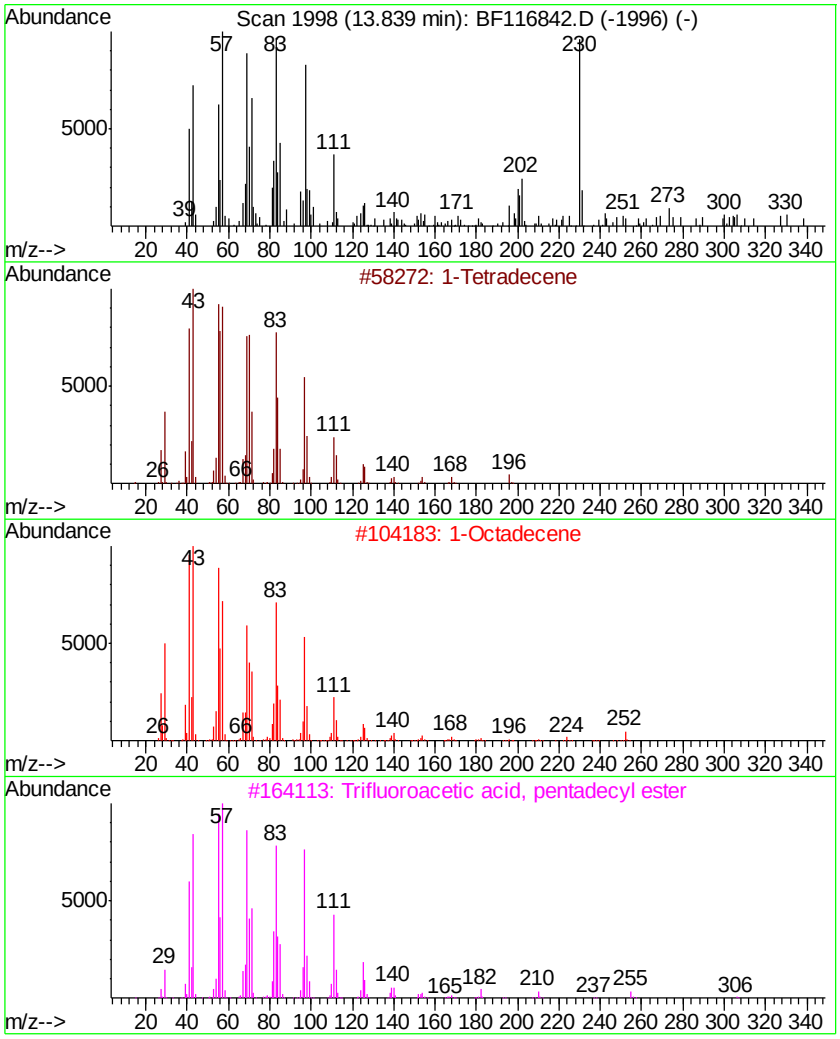
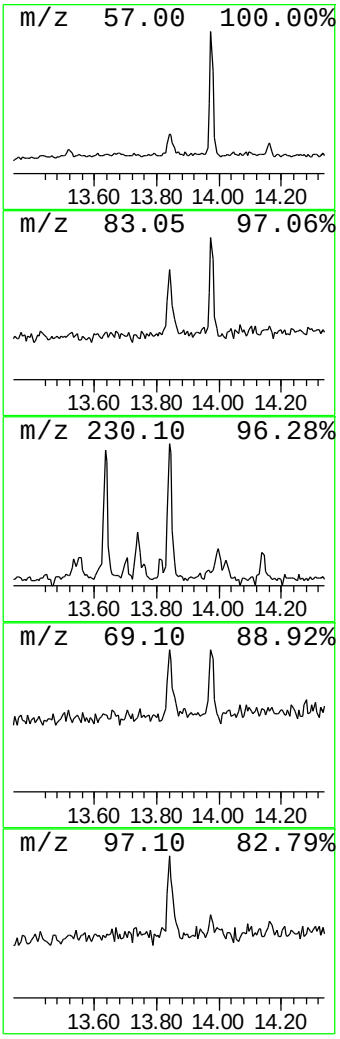
Peak Number 4 1-Tetradecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	5.10 ng	164835	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecene	196	C14H28	001120-36-1	64
2	1-Octadecene	252	C18H36	000112-88-9	64
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	64
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	58





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Instrument : BNA_F
ClientSampleId : T1-1-4-(0-1.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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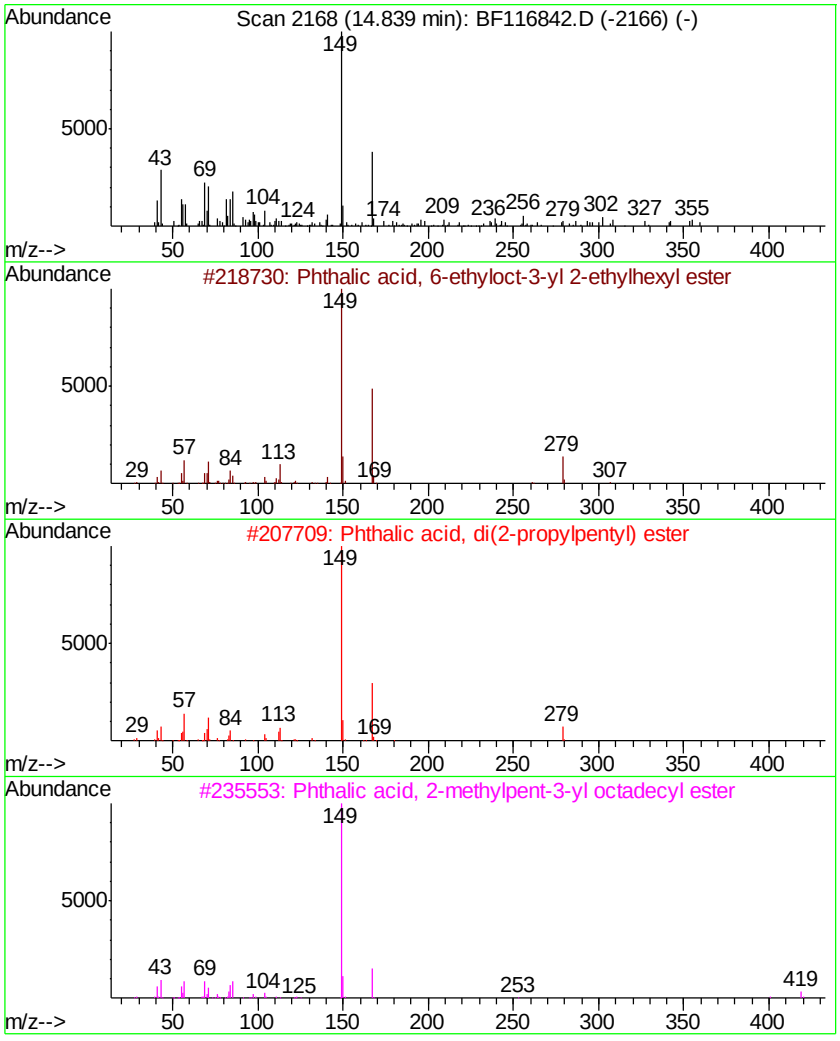
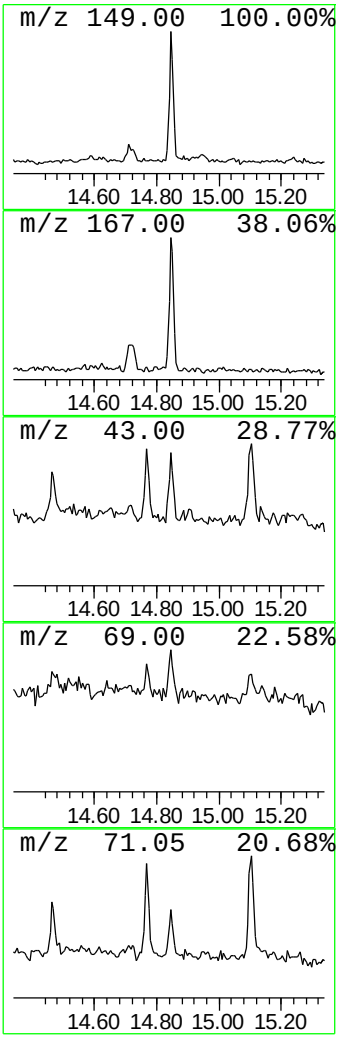
Peak Number 5 Phthalic acid, 6-ethyloct-3... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	3.55 ng	124891	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 6-ethyloct-3-yl 2...	418	C26H42O4	1000315-53-8	83
2	Phthalic acid, di(2-propylpentyl...	390	C24H38O4	1000377-93-5	80
3	Phthalic acid, 2-methylpent-3-yl...	502	C32H54O4	1000356-92-2	72
4	Phthalic acid, dec-2-yl isohexyl...	390	C24H38O4	1000356-94-1	72
5	Phthalic acid, 4-methylpent-2-yl...	376	C23H36O4	1000356-87-9	72





Library Search Compound Report

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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-1-4-(0-1.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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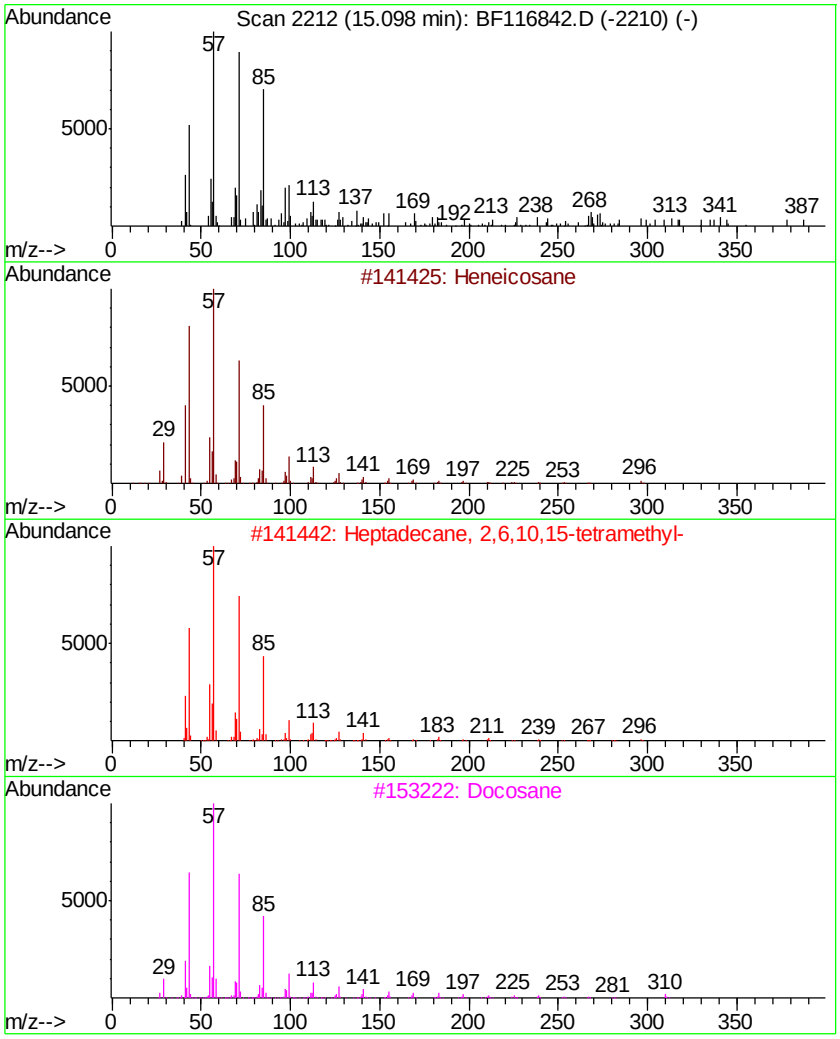
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

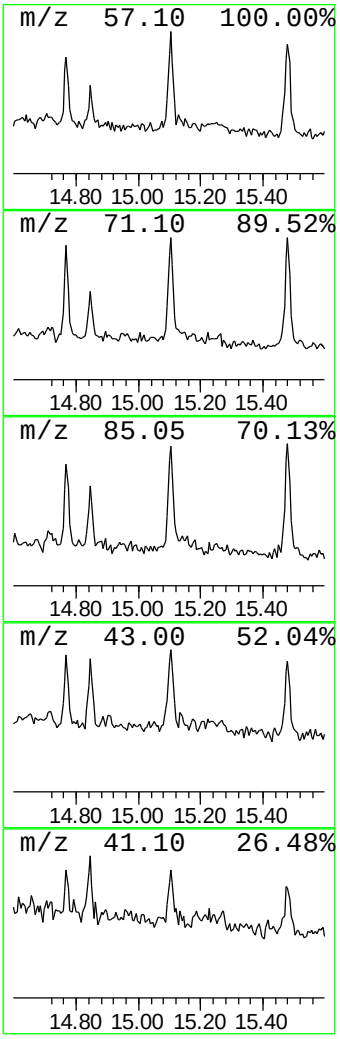
****

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	2.80 ng	98552	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3	Docosane	310	C22H46	000629-97-0	90
4	Tetradecane	198	C14H30	000629-59-4	87
5	Eicosane	282	C20H42	000112-95-8	87





Tentatively Identified Compound (LSC) summary

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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
unknown6.62	6.62	26.3	ng	725782	1	6.85	552271	20.0
n-Hexadecanoic acid	11.89	3.8	ng	149174	4	11.36	778299	20.0
1-Tetradecene	13.84	5.1	ng	164835	5	14.00	646447	20.0
Phthalic acid, 6-...	14.84	3.5	ng	124891	6	15.46	702876	20.0
Heneicosane	15.10	2.8	ng	98552	6	15.46	702876	20.0