LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-COMP

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-BF060716.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	1.690	7	9	17	rVB	99058	215845	5.96%	0.698%
2	1.804	17	19	59	rVB	1689319	3620750	100.00%	11.708%
3	4.879	286	288	296	rBV	93873	138429	3.82%	0.448%
4	5.302	322	325	328	rBV	1580936	2158796	59.62%	6.980%
5	6.365	415	418	421	rBV	1770853	2114632	58.40%	6.838%
6	6.490	426	429	431	rBV	2125039	2417944	66.78%	7.818%
7	6.719	447	449	451	rBV	946030	834337	23.04%	2.698%
8	6.879	460	463	465	rVB	1570055	1945025	53.72%	6.289%
9	7.290	496	499	501	rBV	1554303	1646467	45.47%	5.324%
10	7.999	559	561	564	rBV	953034	1076685	29.74%	3.481%
11	9.085	653	656	658	rBV	2819856	2663005	73.55%	8.611%
12	9.473	688	690	692	rBV	445029	590462	16.31%	1.909%
13	9.611	701	702	705	rBV	56984	51201	1.41%	0.166%
14	9.691	707	709	712	rBV	38633	44037	1.22%	0.142%
15	9.759	712	715	717	rBV	932648	1225461	33.85%	3.963%
16	10.193	752	753	755	rVB	130310	99182	2.74%	0.321%
17	10.411	769	772	775	rBV	45797	74500	2.06%	0.241%
18	10.536	781	783	786	rBV2	1214940	1470761	40.62%	4.756%
19	10.662	792	794	799	rBV	150449	168008	4.64%	0.543%
20	11.108	832	833	835	rBV	78004	70987	1.96%	0.230%
21	11.234	842	844	845	rBV	1281139	1165198	32.18%	3.768%
22	11.256	845	846	847	rVV	71552	51274	1.42%	0.166%
23	11.302	847	850	852	rVB2	54357	63838	1.76%	0.206%
24	11.771	889	891	893	rBV2	48871	79722	2.20%	0.258%
25	11.839	895	897	902	rVB	46845	71107	1.96%	0.230%
26	12.274	932	935	937	rBV2	20665	39097	1.08%	0.126%
27	12.365	942	943	945	rVB	42067	36377	1.00%	0.118%
28	12.434	947	949	951	rBV	192065	202967	5.61%	0.656%
29	12.662	966	969	973	rBV	277148	280075	7.74%	0.906%
30	12.822	980	983	985	rVB	1641431	2232849	61.67%	7.220%
31	12.994	994	998	1000	rVB	30717	64570	1.78%	0.209%
32	13.062	1000	1004	1005	rBV3	25029	50352	1.39%	0.163%
33	13.097	1005	1007	1011	rBV2	45112	61196	1.69%	0.198%
34	13.188	1011	1015	1016	rBV	32009	41809	1.15%	0.135%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-COMP

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.394	1027	1033	1036	rBV3	26510	56444	1.56%	0.183%
36	13.611	1049	1052	1053	rBV	26817	36777	1.02%	0.119%
37	13.714	1059	1061	1066	rBV2	150036	218644	6.04%	0.707%
38	13.862	1071	1074	1075	rBV2	868690	993309	27.43%	3.212%
39	14.034	1088	1089	1092	rVB2	40330	46381	1.28%	0.150%
40	14.251	1103	1108	1109	rBV2	32461	60008	1.66%	0.194%
41	14.342	1114	1116	1122	rVB4	88951	209083	5.77%	0.676%
42	14.617	1138	1140	1146	rBV3	47135	118518	3.27%	0.383%
43	14.708	1146	1148	1152	rVV3	23456	55681	1.54%	0.180%
44	14.868	1159	1162	1166	rBV	137159	283027	7.82%	0.915%
45	14.960	1166	1170	1176	rVV2	89406	244755	6.76%	0.791%
46	15.131	1183	1185	1188	rVB	86028	106346	2.94%	0.344%
47	15.188	1188	1190	1193	rVB	107459	151062	4.17%	0.488%
48	15.245	1193	1195	1197	rBV	585933	768550	21.23%	2.485%
49	15.668	1229	1232	1234	rBV	54345	81660	2.26%	0.264%
50	16.571	1307	1311	1314	rBV	66193	132190	3.65%	0.427%
51	16.628	1314	1316	1320	rVB2	21631	40546	1.12%	0.131%
52	16.834	1332	1334	1339	rVB4	25490	55572	1.53%	0.180%
53	16.960	1343	1345	1351	rVB	49381	95244	2.63%	0.308%
54	17.074	1351	1355	1363	rVB6	12800	47370	1.31%	0.153%
55	18.983	1519	1522	1532	rVB2	13713	58081	1.60%	0.188%

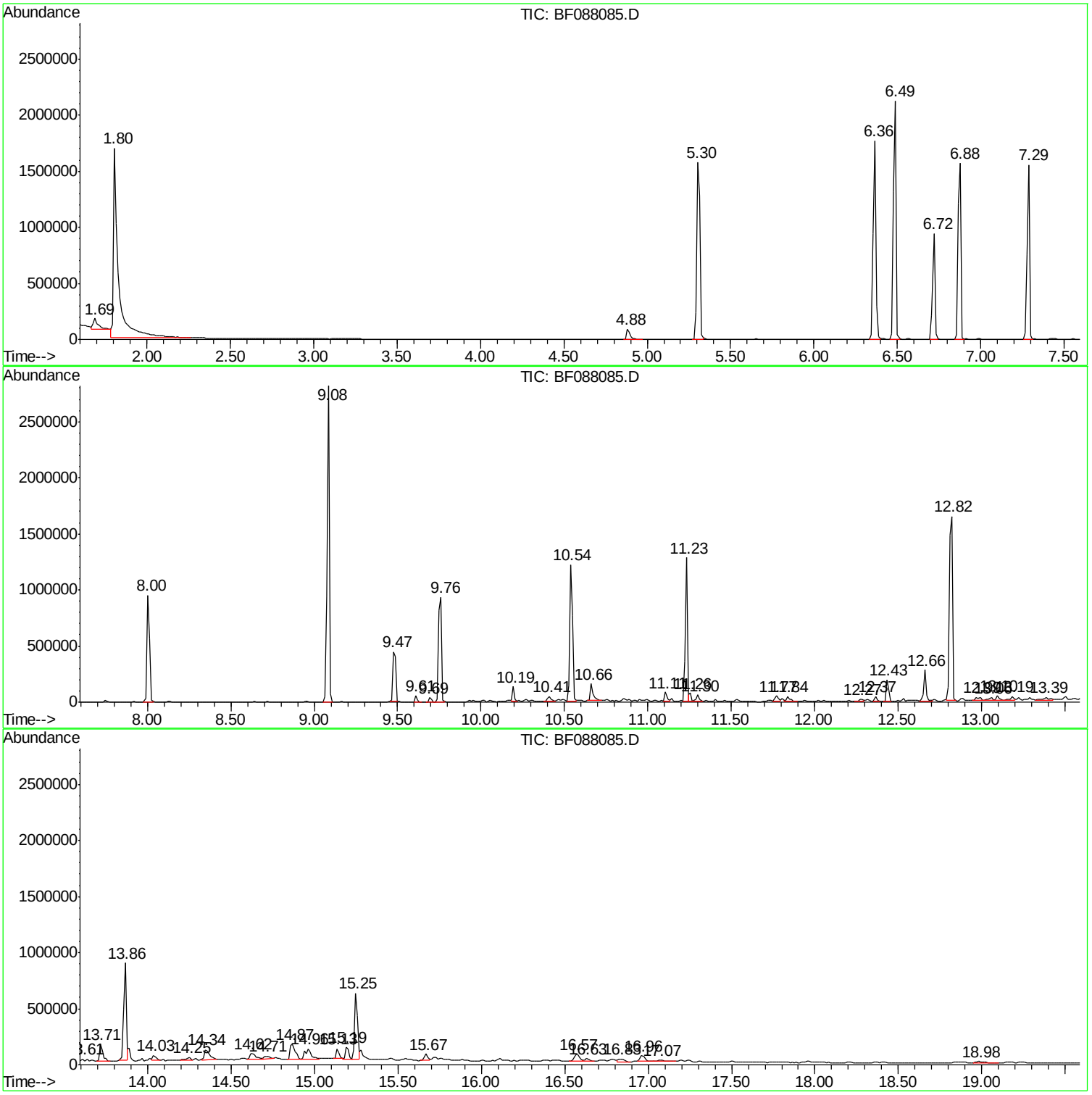
Sum of corrected areas: 30926193

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

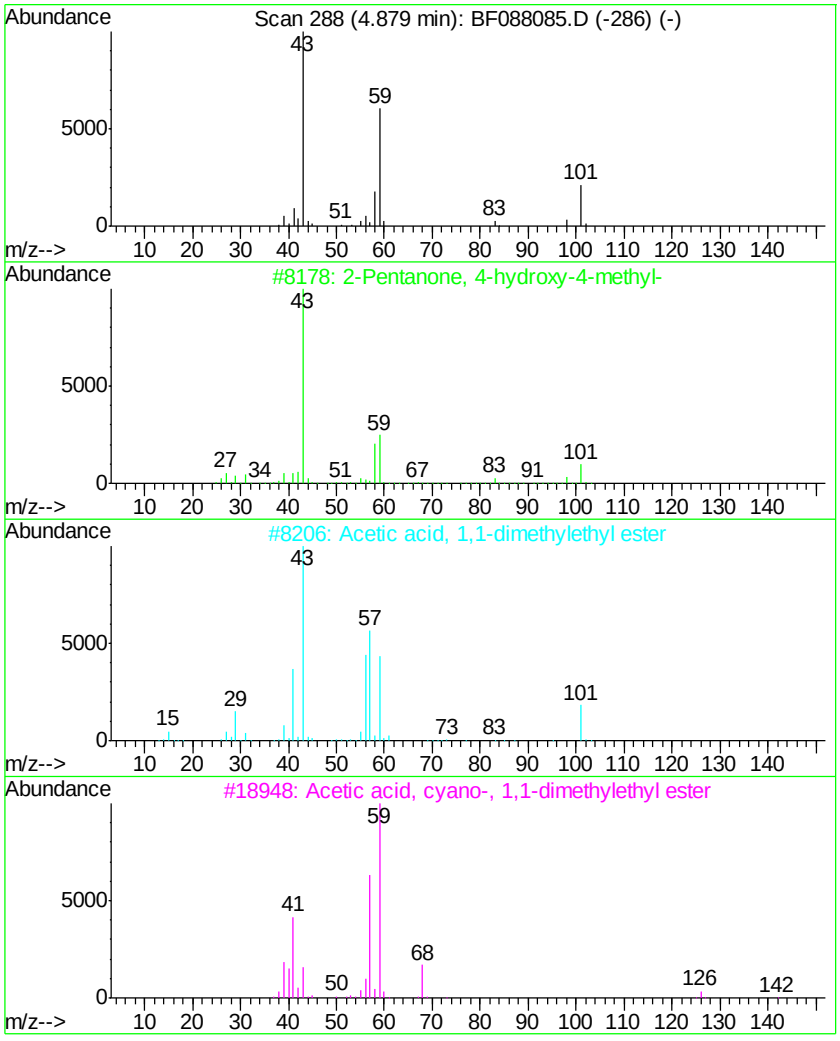
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

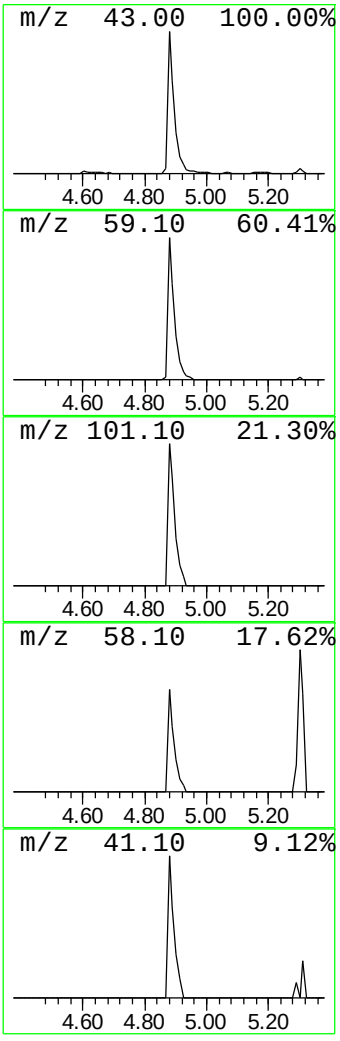
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	3.32 ng	138429	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

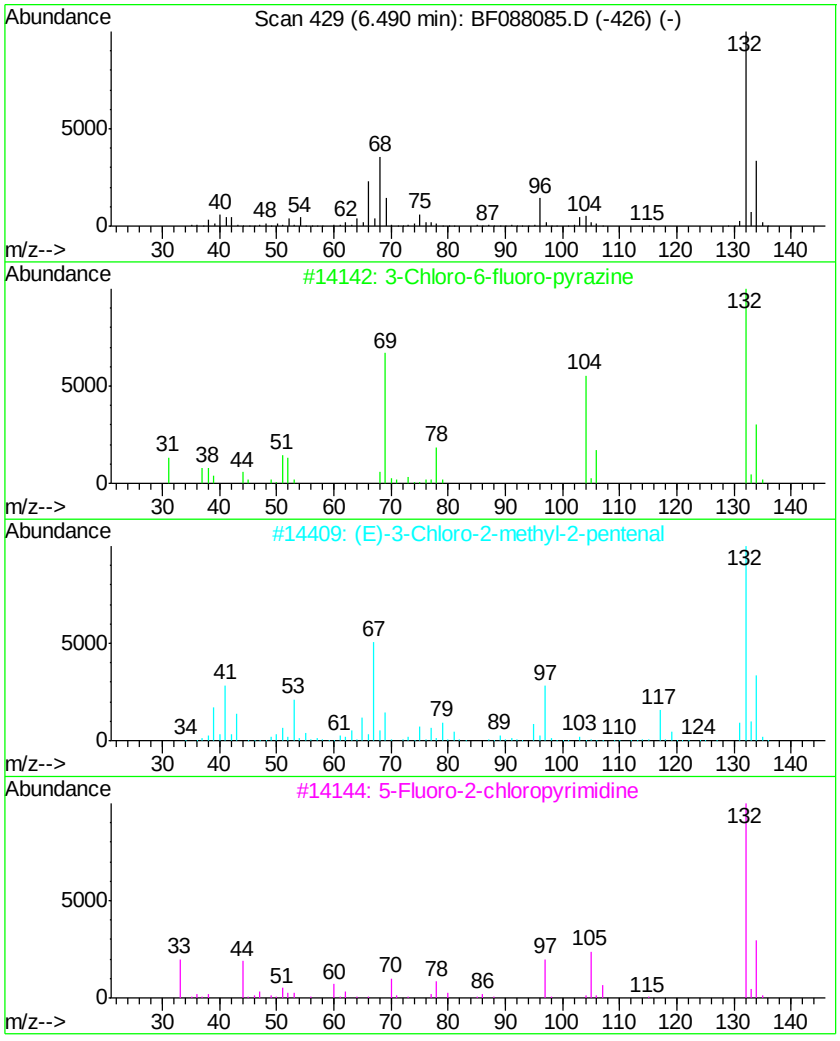
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

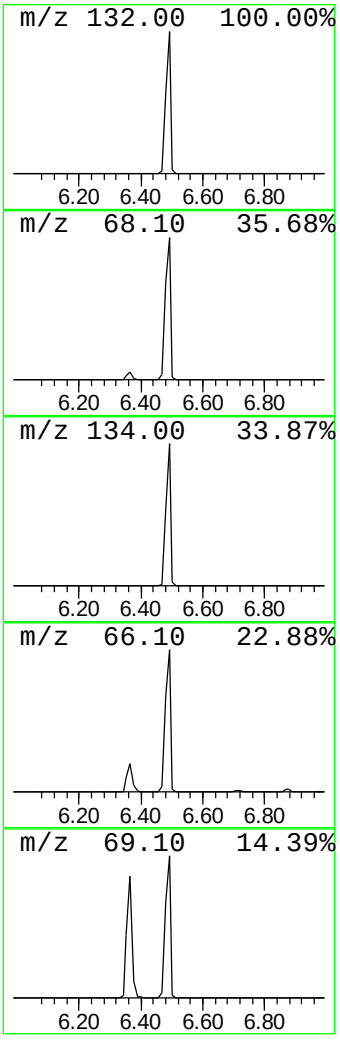
****

Peak Number 4 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	57.96 ng	2417940	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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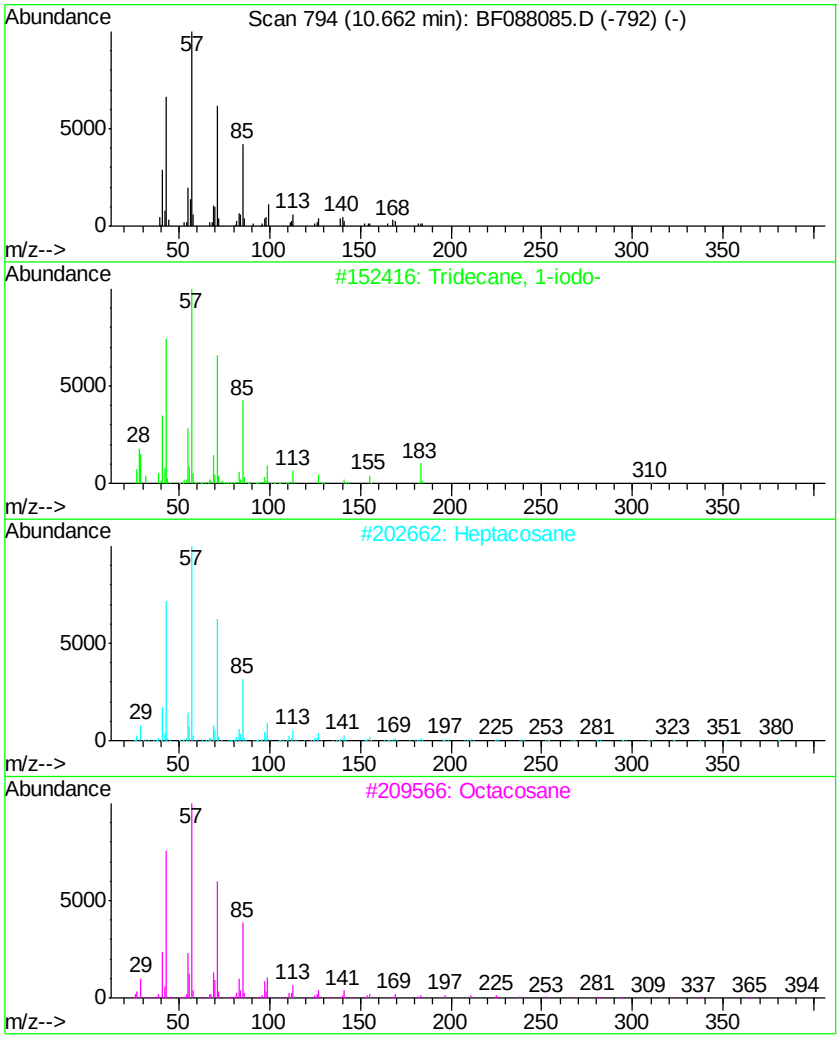
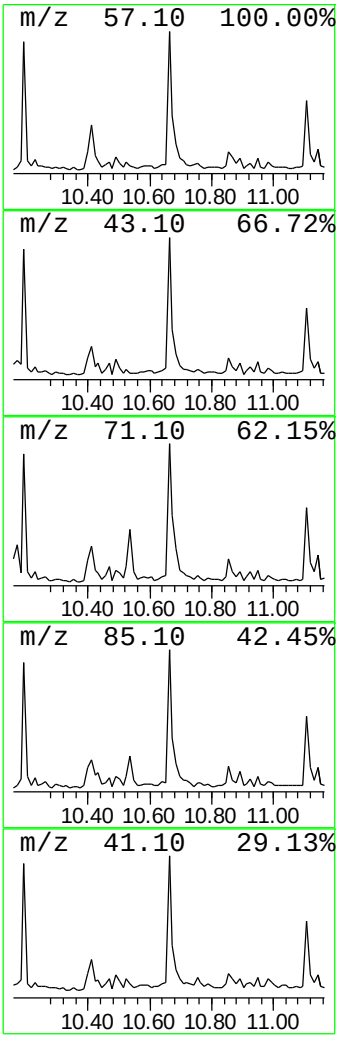
Peak Number 6 Tridecane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.88 ng	168008	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
2	Heptacosane	380	C27H56	000593-49-7	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
5	Tetradecane	198	C14H30	000629-59-4	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

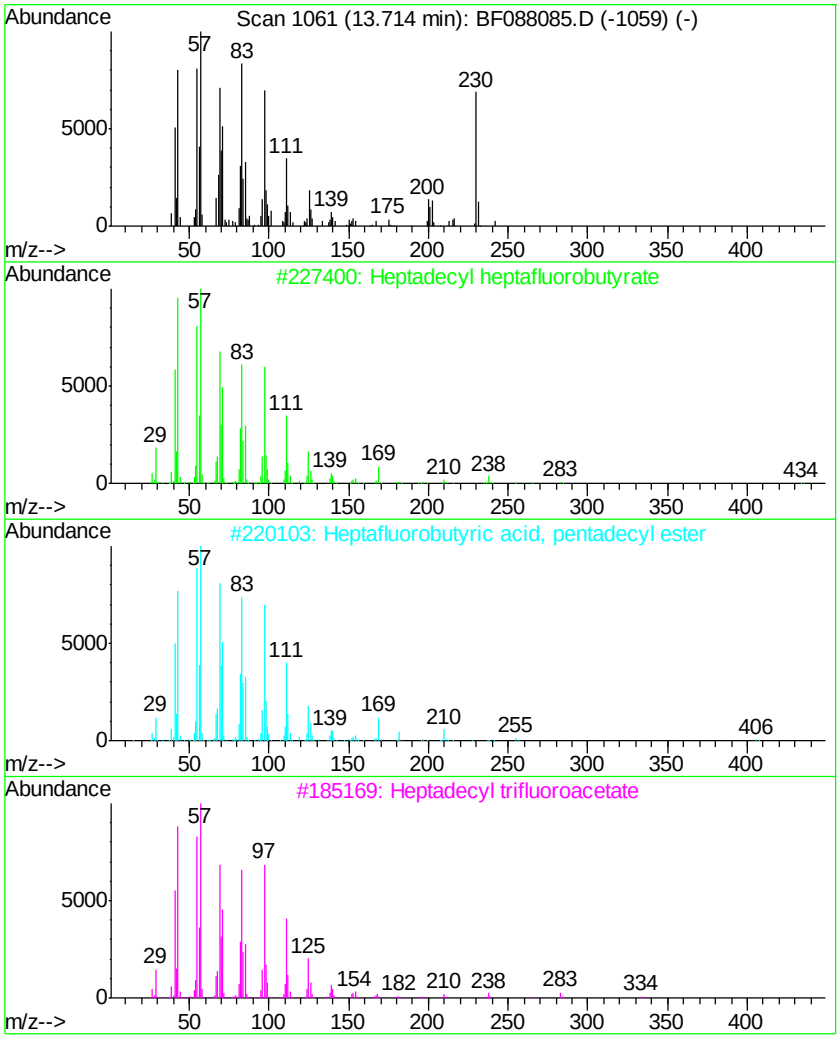
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

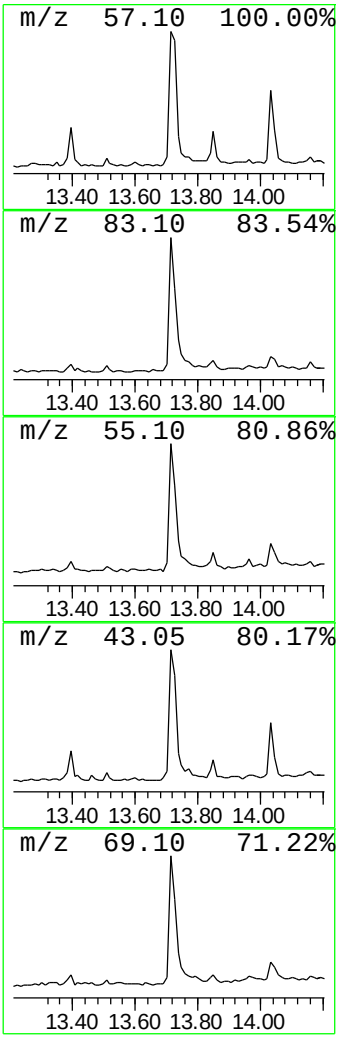
****

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	4.40 ng	218644	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

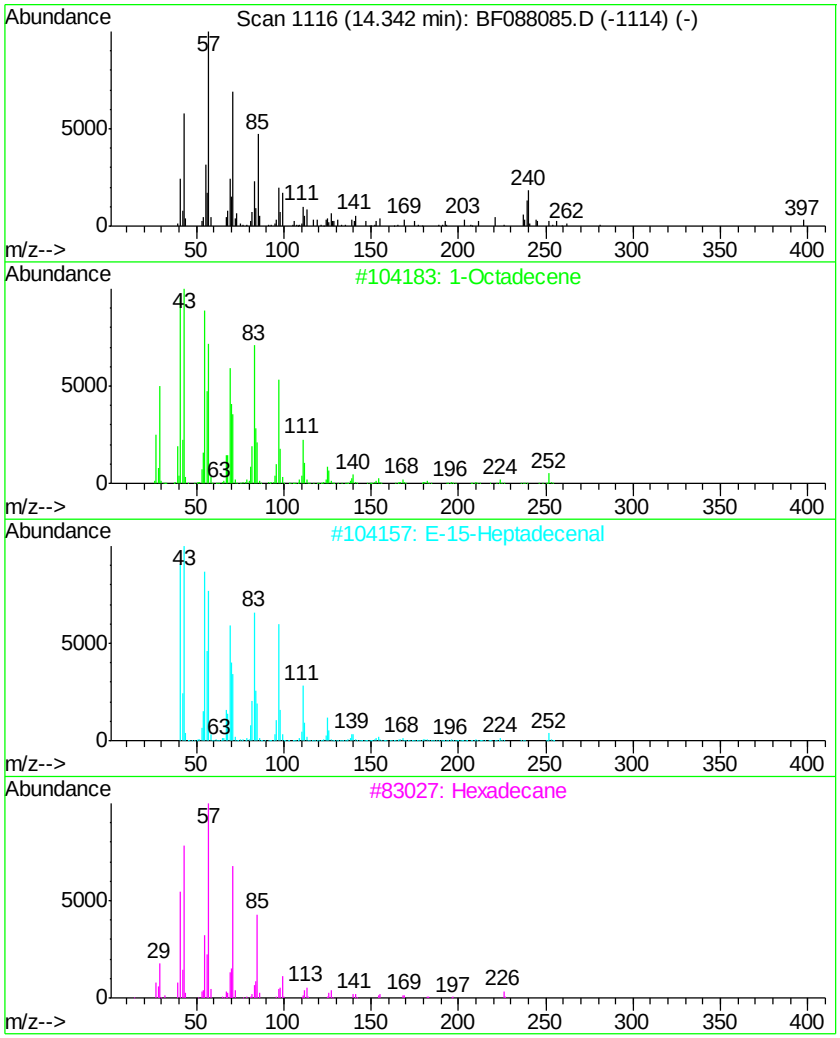
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

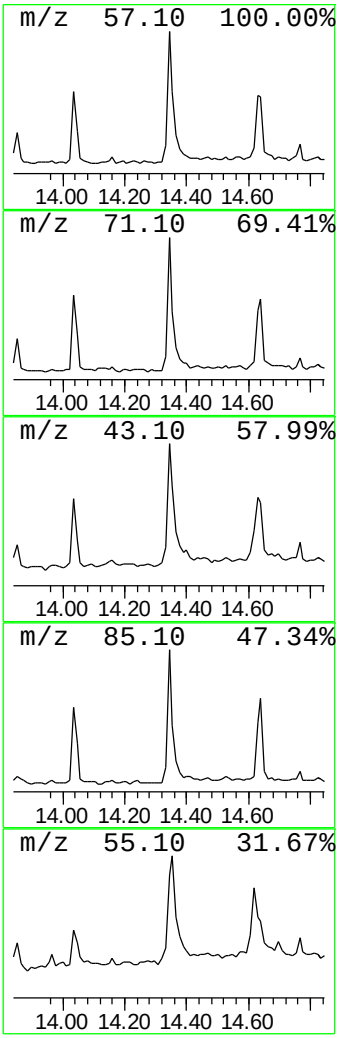
****

Peak Number 8 1-Octadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	4.21 ng	209083	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	92
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	92
3	Hexadecane	226	C16H34	000544-76-3	89
4	Heptadecane	240	C17H36	000629-78-7	78
5	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	74





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

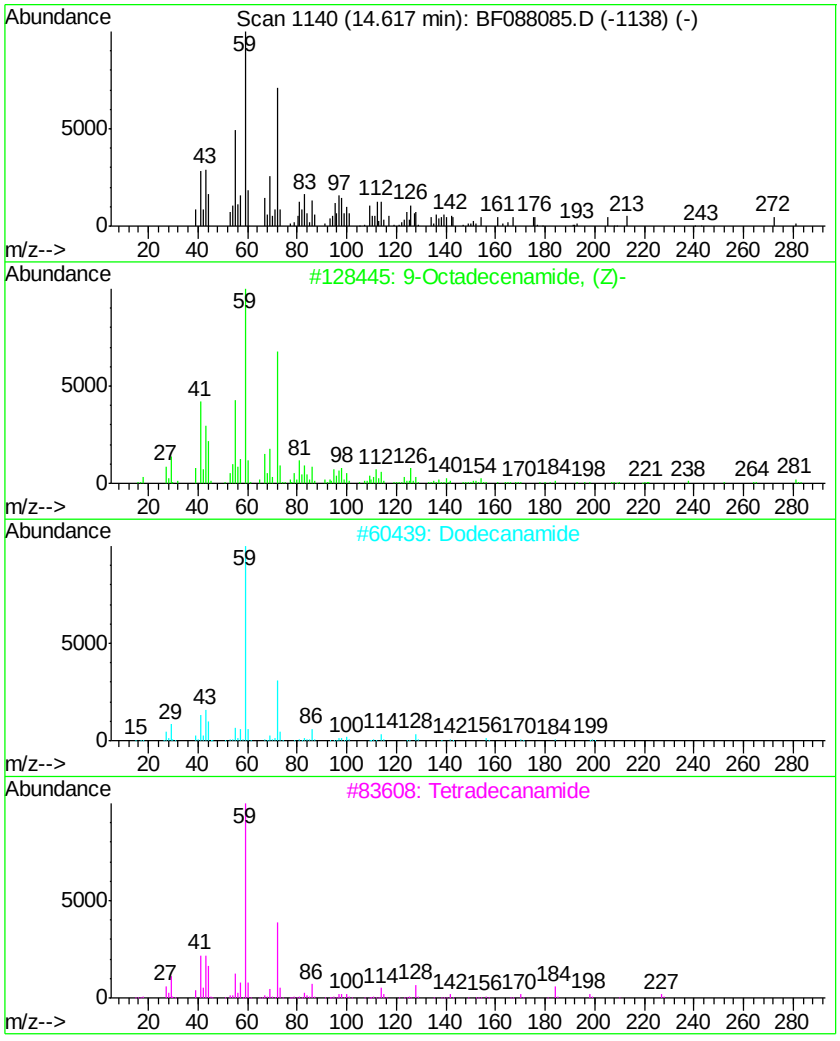
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

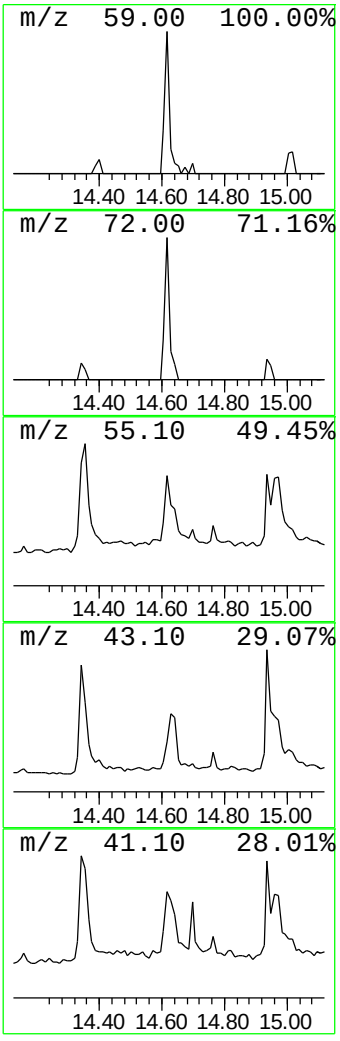
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.08 ng	118518	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	Dodecanamide	199	C12H25NO	001120-16-7	59
3	Tetradecanamide	227	C14H29NO	000638-58-4	59
4	d-Glucosamine	179	C6H13NO5	000090-77-7	50
5	Octanamide	143	C8H17NO	000629-01-6	43





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Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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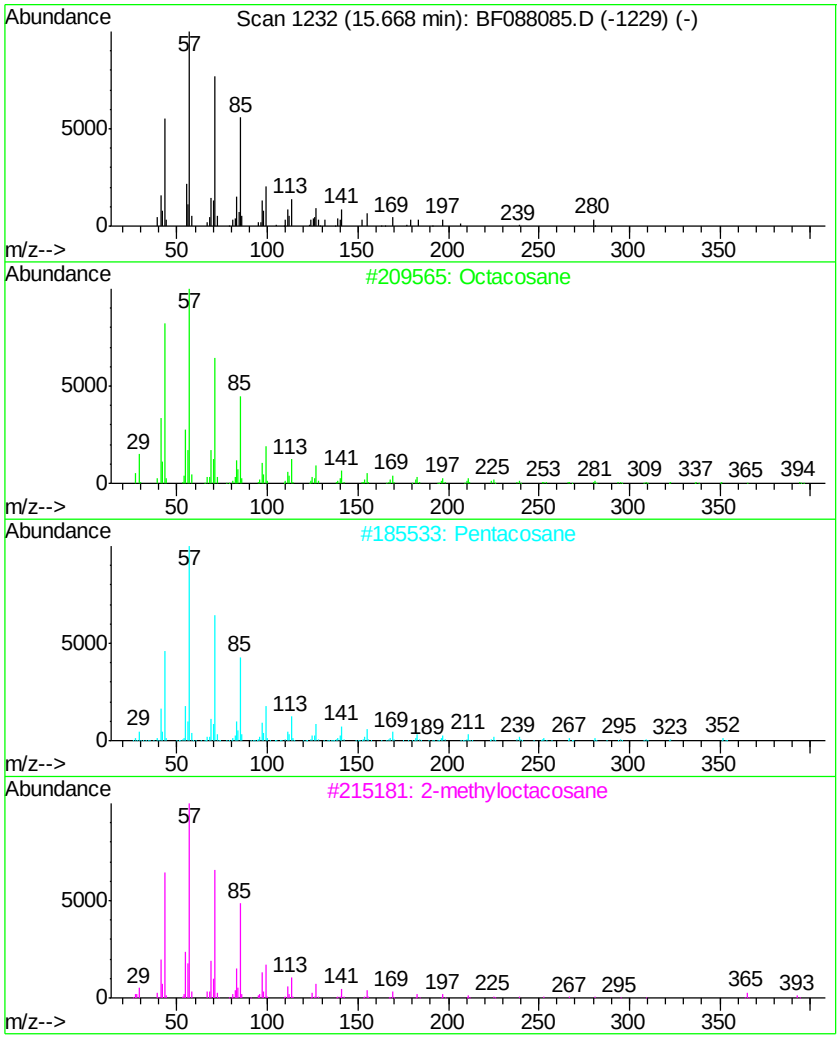
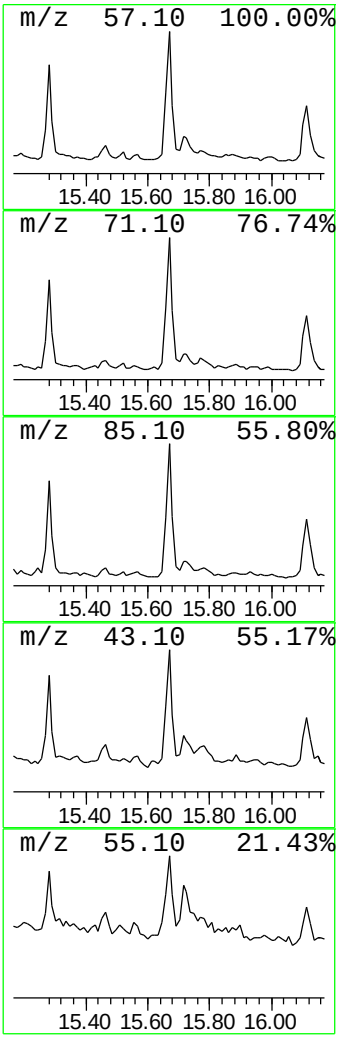
Peak Number 12 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	2.13 ng	81660	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061616\
Data File : BF088085.D
Acq On : 16 Jun 2016 19:48
Operator : UM/SJ
Sample : H3571-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.88	3.3	ng	138429	1	6.72	834337	20.0
unknown6.49	6.49	58.0	ng	2417940	1	6.72	834337	20.0
Tridecane, 1-iodo-	10.66	2.9	ng	168008	4	11.23	1165200	20.0
Heptadecyl heptaf...	13.71	4.4	ng	218644	5	13.86	993309	20.0
1-Octadecene	14.34	4.2	ng	209083	5	13.86	993309	20.0
9-Octadecenamide,...	14.62	3.1	ng	118518	6	15.25	768550	20.0
Octacosane	15.67	2.1	ng	81660	6	15.25	768550	20.0