LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

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-BF012218.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	4.928	478	483	490	rBV	79887	116490	2.88%	0.335%
2	5.334	547	552	568	rBV	3714901	3887839	96.06%	11.172%
3	6.369	722	728	739	rBV	3427161	4047459	100.00%	11.630%
4	6.486	744	748	752	rBV	3826458	3831871	94.67%	11.011%
5	6.716	783	787	794	rBV	1275947	1124679	27.79%	3.232%
6	6.869	809	813	822	rBV	3108392	2776093	68.59%	7.977%
7	7.286	879	884	895	rBV	2376342	2442604	60.35%	7.019%
8	7.457	909	913	918	rVB	62961	56453	1.39%	0.162%
9	7.998	1001	1005	1026	rVB	1604452	1493370	36.90%	4.291%
10	9.069	1183	1187	1198	rBV	3051622	3008597	74.33%	8.645%
11	9.145	1198	1200	1203	rVB	67716	54944	1.36%	0.158%
12	9.398	1239	1243	1248	rBV5	28084	42173	1.04%	0.121%
13	9.469	1248	1255	1262	rVB	393082	392019	9.69%	1.126%
14	9.675	1287	1290	1294	rBV	187570	149453	3.69%	0.429%
15	9.751	1295	1303	1306	rVV	1498298	1368522	33.81%	3.932%
16	9.780	1306	1308	1312	rVB	70675	60580	1.50%	0.174%
17	9.904	1325	1329	1332	rBV4	30535	43300	1.07%	0.124%
18	9.998	1341	1345	1348	rVB3	41625	42973	1.06%	0.123%
19	10.174	1372	1375	1378	rVB	237091	173972	4.30%	0.500%
20	10.298	1393	1396	1401	rVB	53598	49173	1.21%	0.141%
21	10.392	1405	1412	1415	rBV	54146	82966	2.05%	0.238%
22	10.539	1434	1437	1447	rBV	1511637	1596355	39.44%	4.587%
23	10.645	1452	1455	1463	rBV	159461	164910	4.07%	0.474%
24	11.092	1528	1531	1535	rBV	61103	58745	1.45%	0.169%
25	11.239	1552	1556	1558	rBV	960615	949350	23.46%	2.728%
26	11.257	1558	1559	1565	rVV	405228	354454	8.76%	1.019%
27	11.310	1565	1568	1572	rVB	94948	96005	2.37%	0.276%
28	11.474	1592	1596	1600	rBV	46975	57762	1.43%	0.166%
29	11.739	1637	1641	1643	rBV	56205	48465	1.20%	0.139%
30	11.769	1643	1646	1648	rVV	56994	49482	1.22%	0.142%
31	11.851	1656	1660	1662	rBV	91746	93127	2.30%	0.268%
32	12.451	1758	1762	1766	rVB	622211	547625	13.53%	1.574%
33	12.680	1795	1801	1806	rBV	544865	573322	14.16%	1.647%
34	12.821	1819	1825	1828	rBV	1962473	1785692	44.12%	5.131%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

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-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.898	1835	1838	1841	rVB3	33094	44345	1.10%	0.127%
36	12.986	1849	1853	1854	rBV4	38629	46755	1.16%	0.134%
37	13.004	1854	1856	1859	rVB	69142	72050	1.78%	0.207%
38	13.074	1865	1868	1870	rBV	55048	47246	1.17%	0.136%
39	13.715	1974	1977	1986	rVB3	189148	270344	6.68%	0.777%
40	13.880	2000	2005	2007	rBV2	890119	1014142	25.06%	2.914%
41	13.904	2007	2009	2015	rVB	254655	213887	5.28%	0.615%
42	14.339	2080	2083	2087	rBV3	79879	116314	2.87%	0.334%
43	14.898	2176	2178	2181	rBV	119126	141176	3.49%	0.406%
44	14.951	2184	2187	2191	rVB	354047	360378	8.90%	1.036%
45	15.251	2235	2238	2241	rBV	121407	136259	3.37%	0.392%
46	15.309	2244	2248	2253	rVV	450172	532263	13.15%	1.529%
47	15.715	2315	2317	2322	rVB	147569	185081	4.57%	0.532%

Sum of corrected areas: 34801064

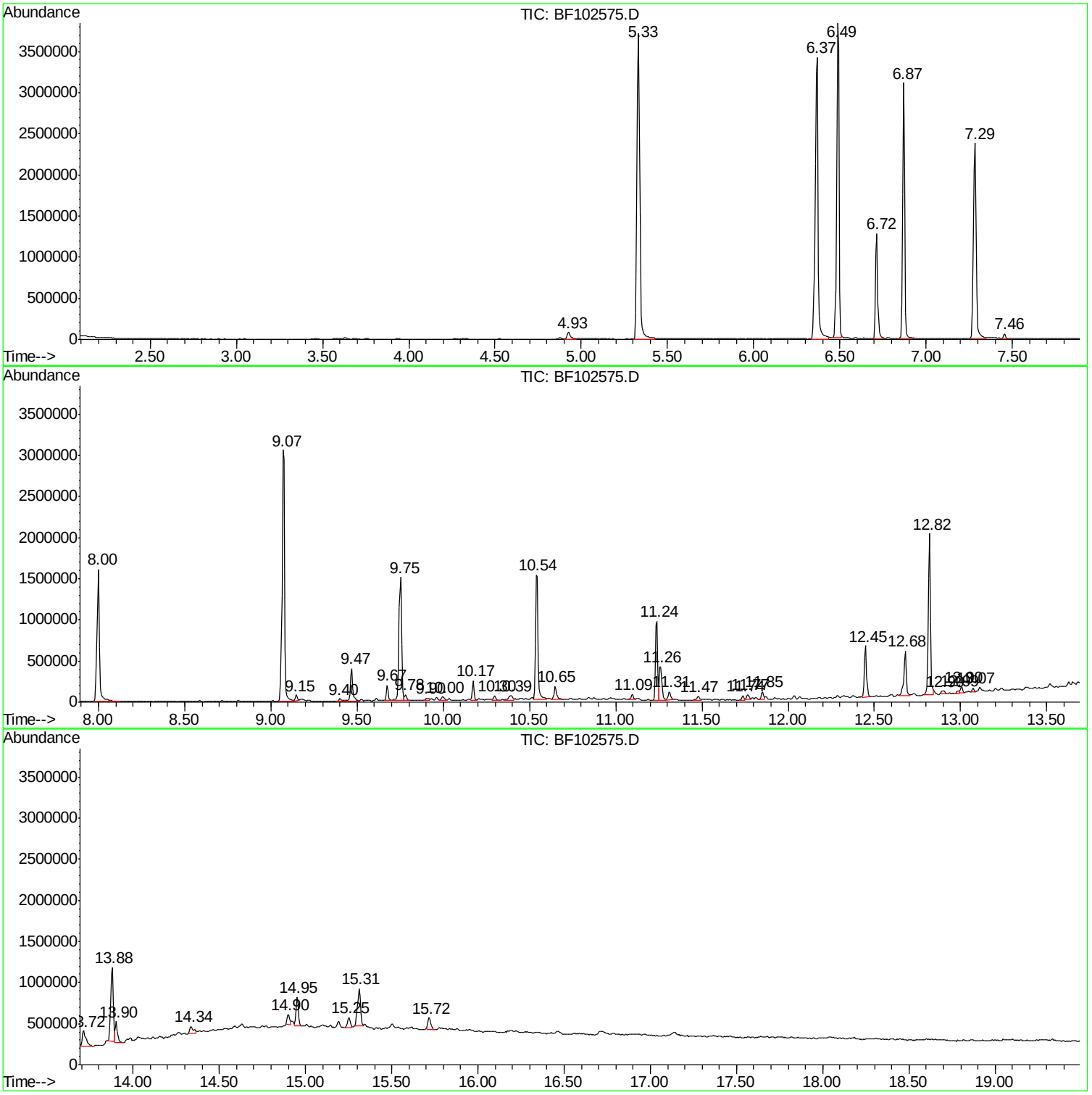
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

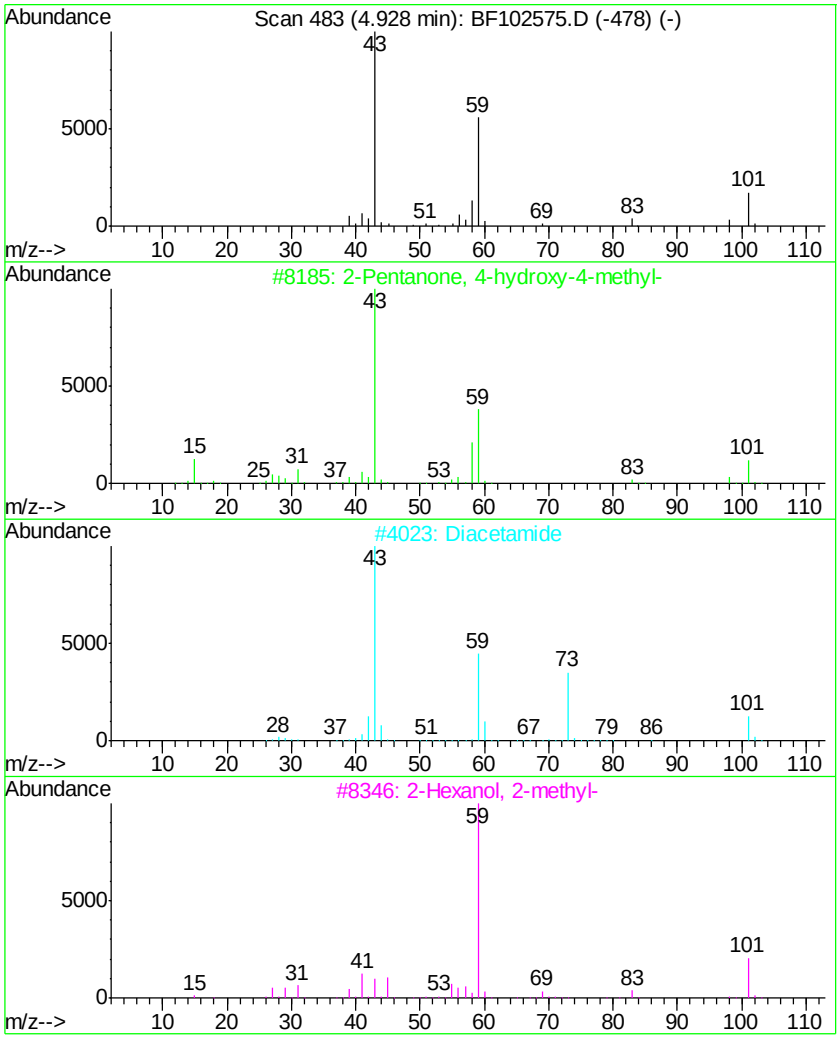
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

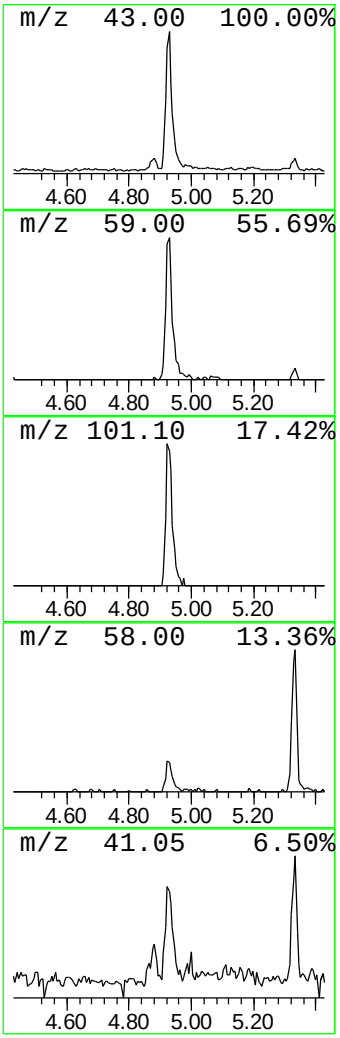
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.07 ng	116490	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	Diacetamide	101	C4H7NO2	000625-77-4	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4	1,2-Butanediol	90	C4H10O2	000584-03-2	37
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

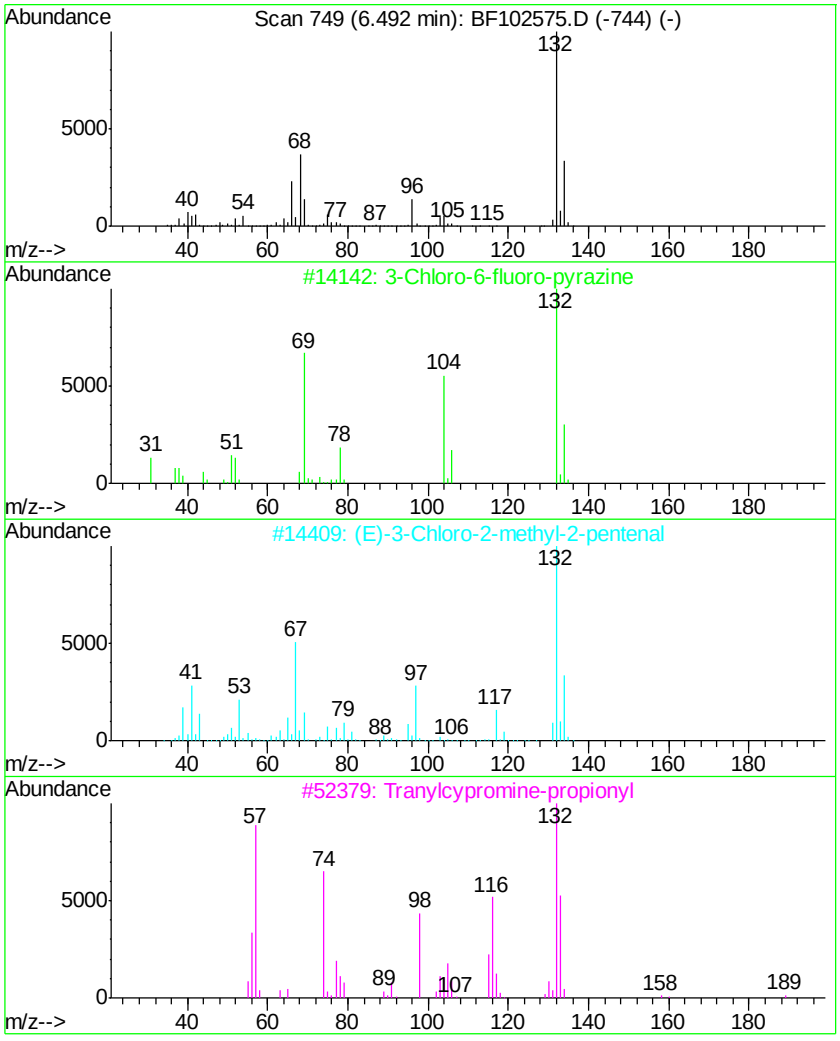
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

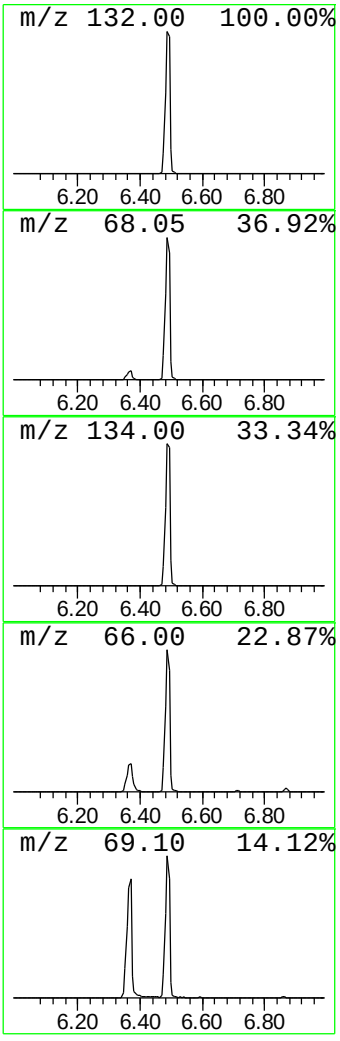
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	68.14 ng	3831870	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

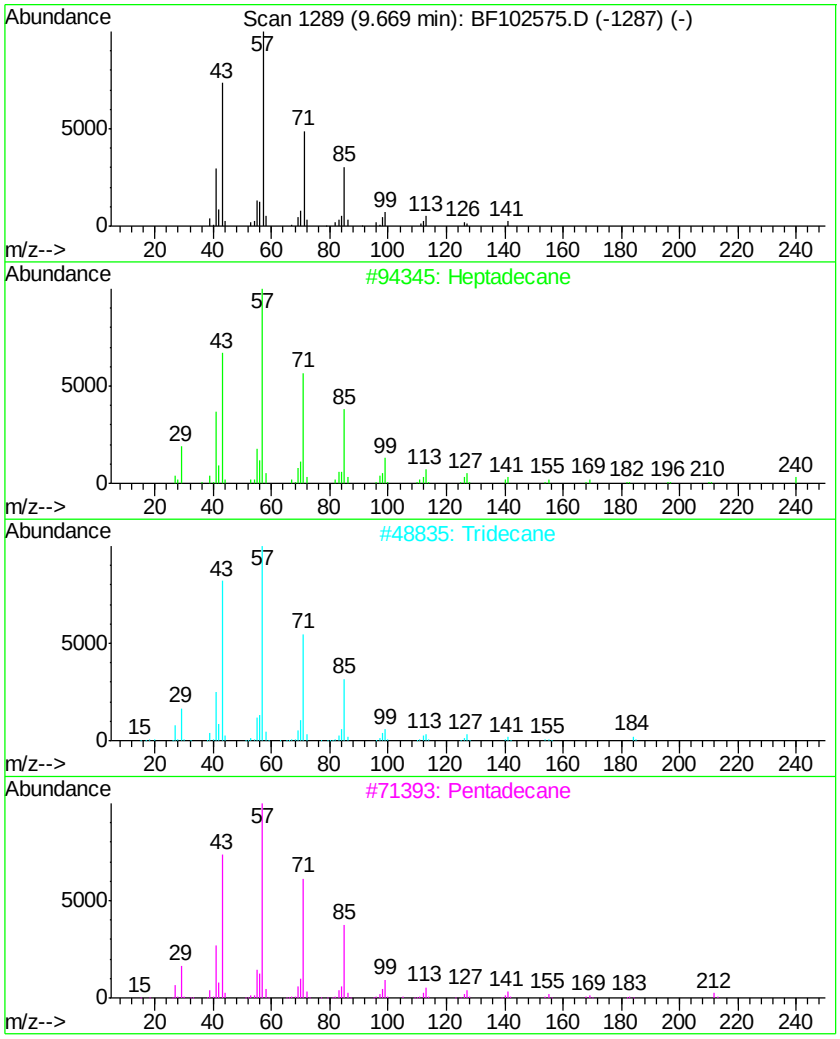
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

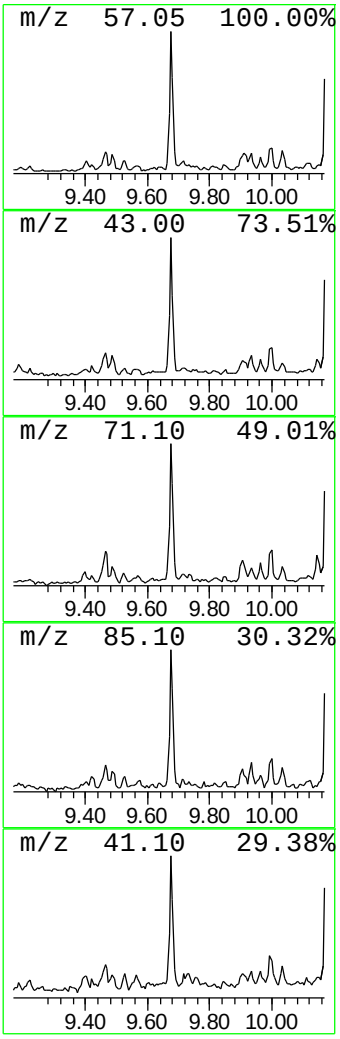
****

Peak Number 4 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.67	2.18 ng	149453	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tridecane	184	C13H28	000629-50-5	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tetradecane	198	C14H30	000629-59-4	90
5	Hexadecane	226	C16H34	000544-76-3	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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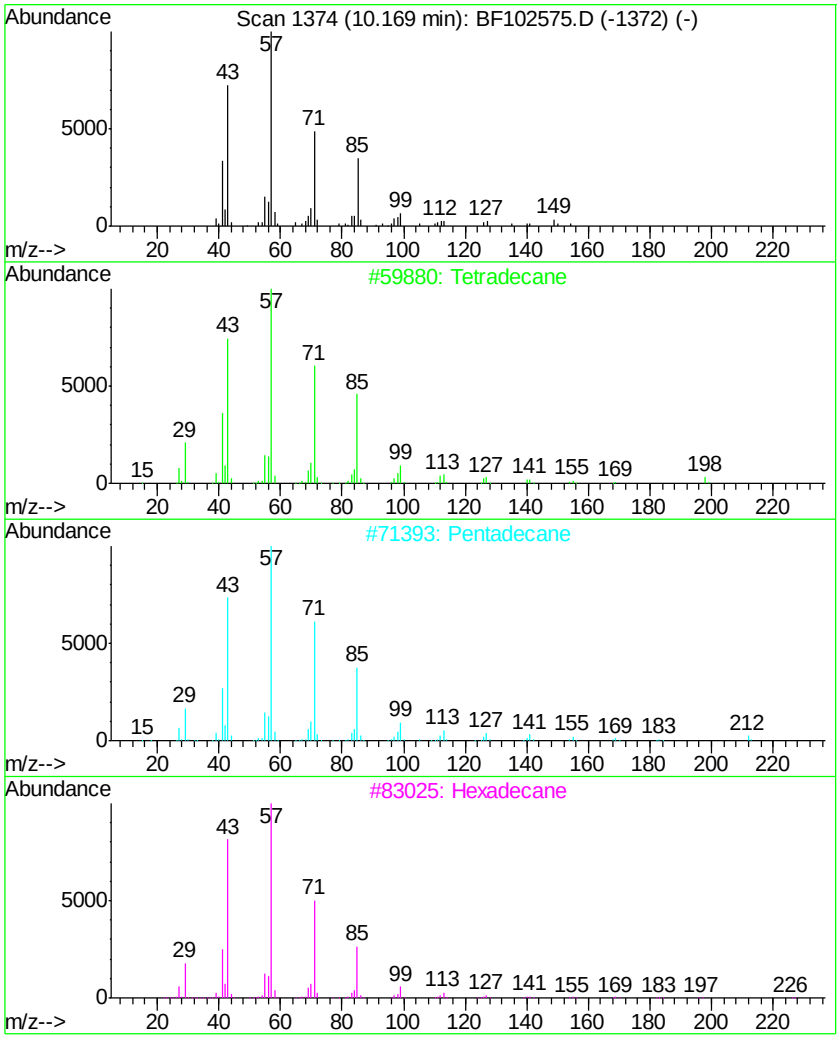
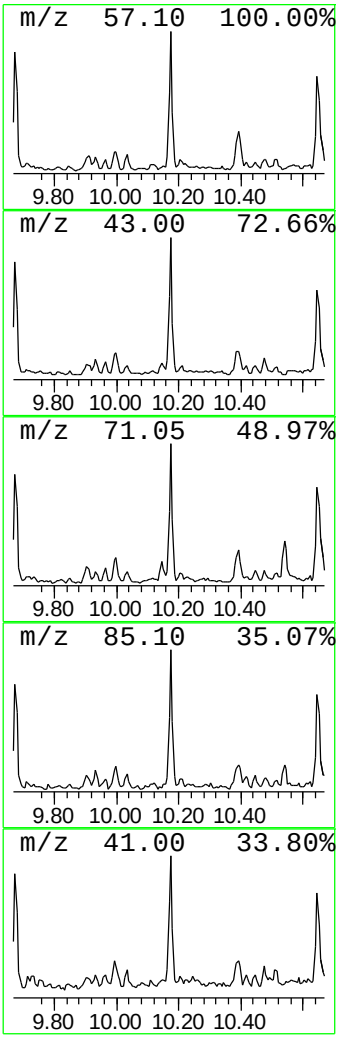
Peak Number 5 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.17	2.54 ng	173972	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
5	Heptadecane	240	C17H36	000629-78-7	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

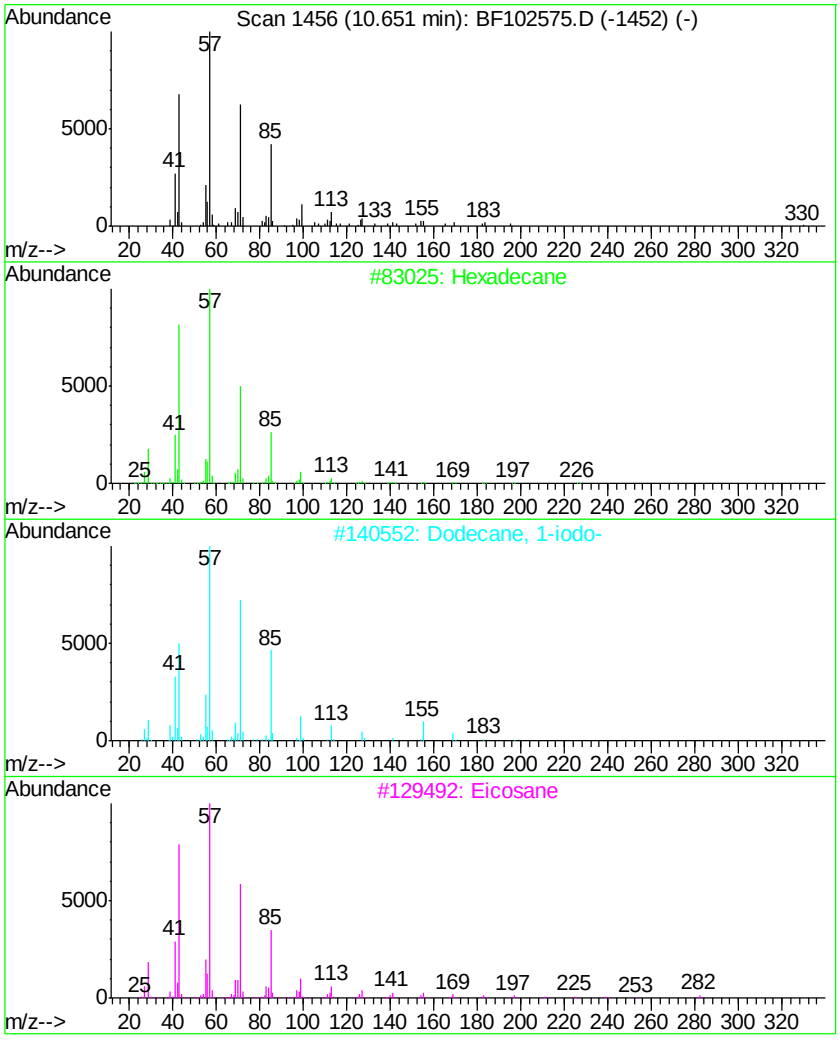
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

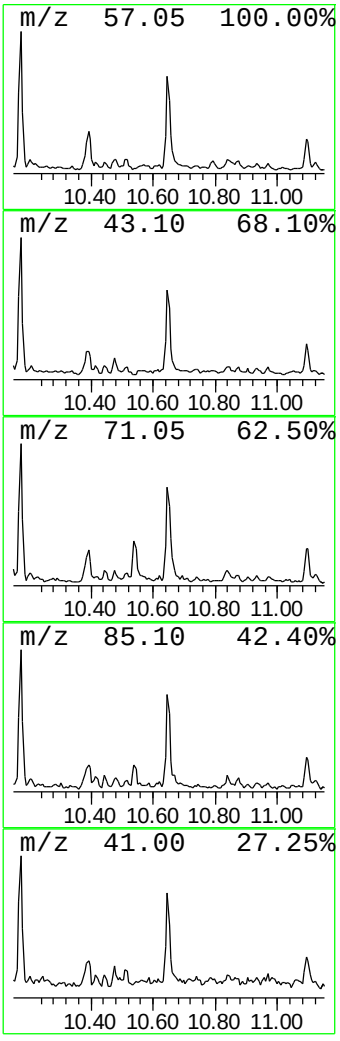
****

Peak Number 6 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	3.47 ng	164910	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Eicosane	282	C20H42	000112-95-8	86
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
5	Nonane, 5-butyl-	184	C13H28	017312-63-9	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

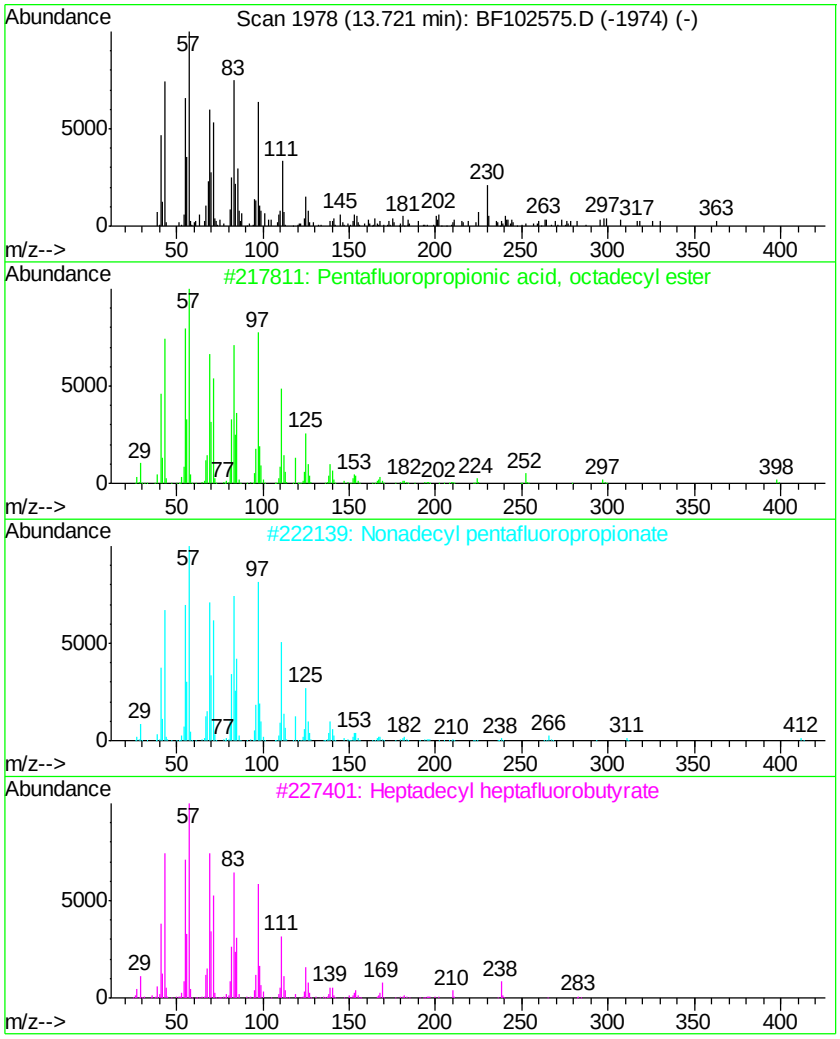
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

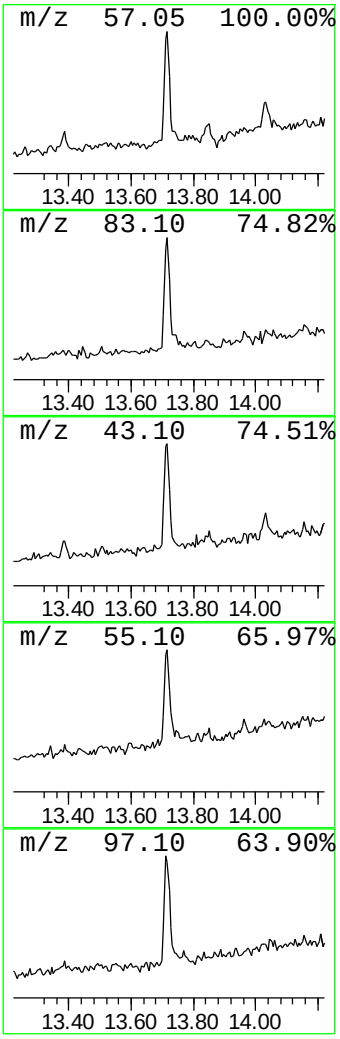
****

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	5.33 ng	270344	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	83
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

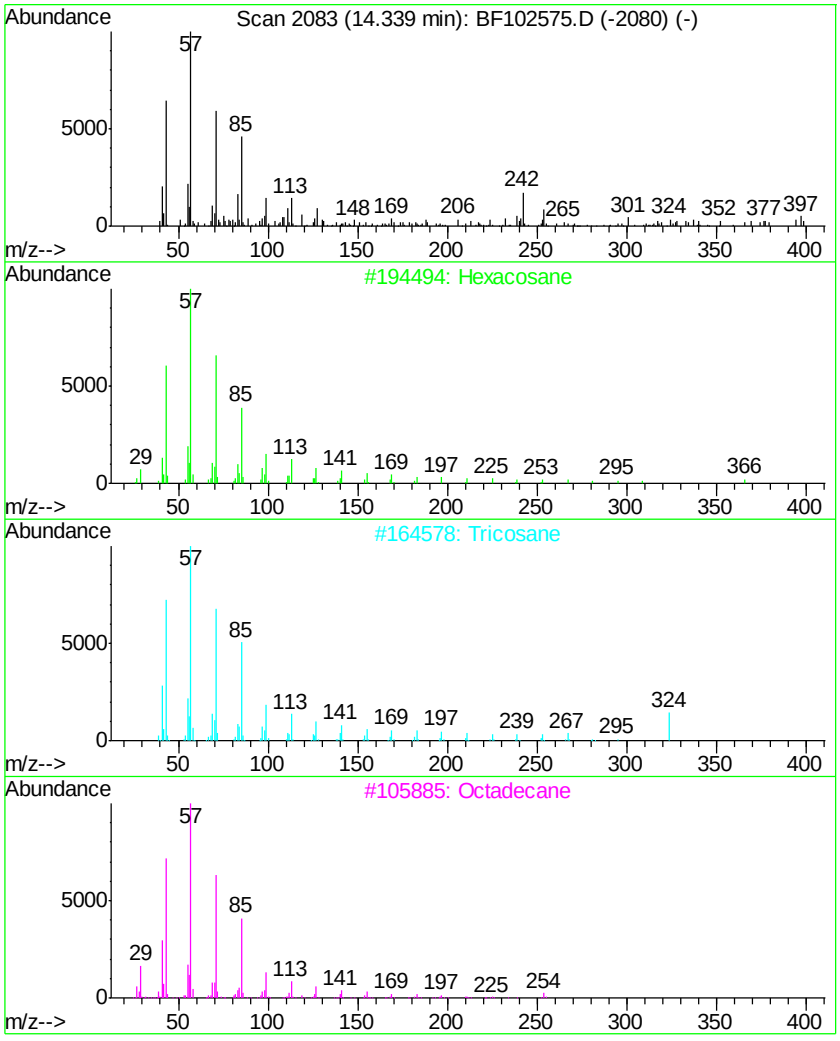
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

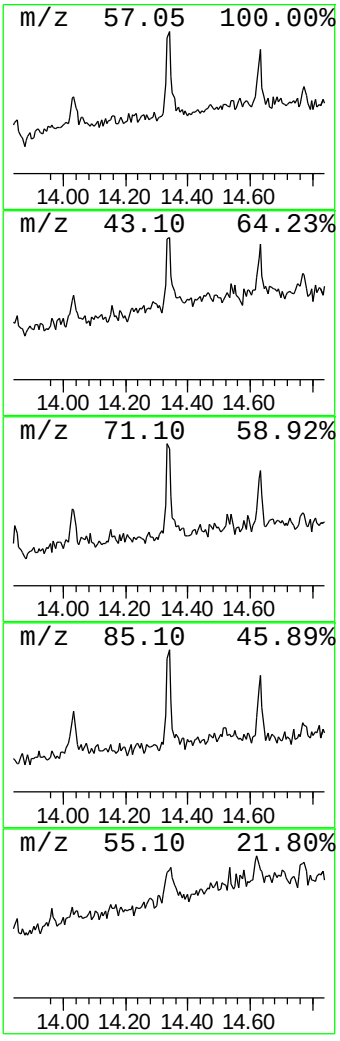
****

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.29 ng	116314	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Tricosane	324	C23H48	000638-67-5	70
3	Octadecane	254	C18H38	000593-45-3	62
4	Heptadecane	240	C17H36	000629-78-7	58
5	Octacosane	394	C28H58	000630-02-4	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

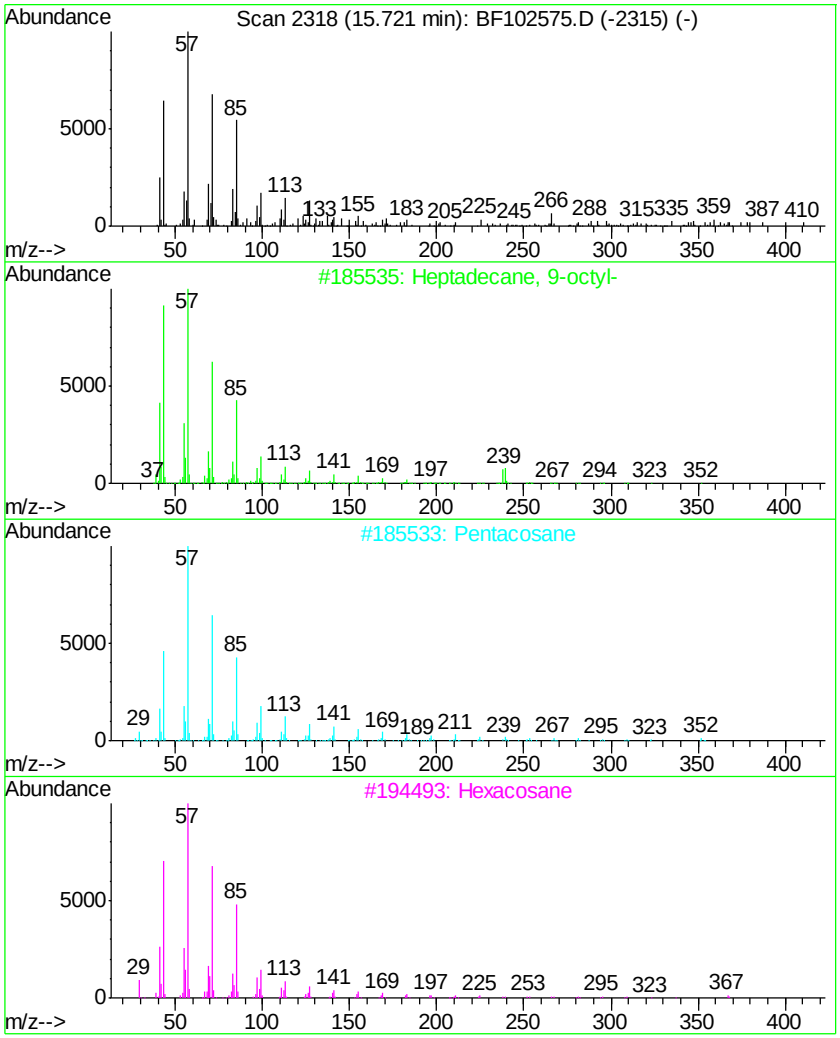
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

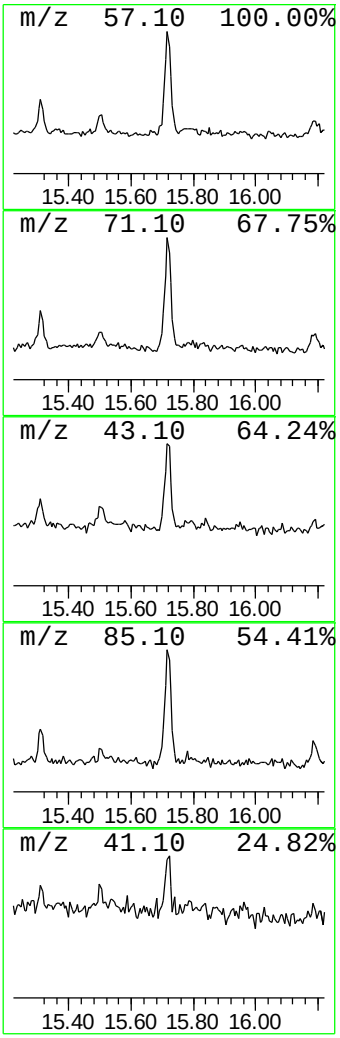
****

Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	6.95 ng	185081	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2	Pentacosane	352	C25H52	000629-99-2	93
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012818\
Data File : BF102575.D
Acq On : 28 Jan 2018 23:18
Operator : SJ/JU
Sample : J1290-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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...	4.93	2.1	ng	116490	1	6.72	1124680	20.0
unknown6.49	6.49	68.1	ng	3831870	1	6.72	1124680	20.0
Heptadecane	9.67	2.2	ng	149453	3	9.75	1368520	20.0
Tetradecane	10.17	2.5	ng	173972	3	9.75	1368520	20.0
Hexadecane	10.65	3.5	ng	164910	4	11.24	949350	20.0
Pentafluoropropio...	13.72	5.3	ng	270344	5	13.88	1014140	20.0
Hexacosane	14.34	2.3	ng	116314	5	13.88	1014140	20.0
Heptadecane, 9-oc...	15.72	7.0	ng	185081	6	15.31	532263	20.0