LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

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-BF102318.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	2.304	31	37	45	rVB	429164	603242	21.18%	2.462%
2	5.204	527	530	543	rVB	87024	129720	4.55%	0.529%
3	5.587	590	595	598	rBV	2484139	2410648	84.64%	9.838%
4	6.581	759	764	775	rBV	2183618	2686529	94.32%	10.963%
5	6.728	784	789	792	rBV	2699042	2598294	91.23%	10.603%
6	6.951	824	827	831	rBV	546372	498522	17.50%	2.034%
7	7.110	850	854	857	rBV	2147671	1926426	67.64%	7.862%
8	7.516	918	923	937	rBV	1422846	1651148	57.97%	6.738%
9	8.239	1041	1046	1057	rBV	606715	656252	23.04%	2.678%
10	9.310	1223	1228	1231	rBV	3005667	2848207	100.00%	11.623%
11	9.704	1290	1295	1304	rBV	287500	276266	9.70%	1.127%
12	9.998	1340	1345	1355	rBV	760075	742392	26.07%	3.030%
13	10.786	1475	1479	1491	rBV	1660699	1665142	58.46%	6.795%
14	11.486	1594	1598	1606	rBV	778664	733444	25.75%	2.993%
15	11.827	1652	1656	1660	rBV	50889	68663	2.41%	0.280%
16	12.033	1687	1691	1695	rVB	38945	48379	1.70%	0.197%
17	12.510	1768	1772	1775	rBV3	32310	38246	1.34%	0.156%
18	12.927	1839	1843	1850	rVB3	23579	38404	1.35%	0.157%
19	13.068	1863	1867	1871	rBV	2455432	2381201	83.60%	9.717%
20	13.621	1956	1961	1963	rBV2	27010	29162	1.02%	0.119%
21	13.945	2012	2016	2020	rBV	165861	176454	6.20%	0.720%
22	13.986	2021	2023	2030	rVB	26885	35807	1.26%	0.146%
23	14.133	2044	2048	2054	rVB	545331	497897	17.48%	2.032%
24	14.262	2064	2070	2077	rVB2	73389	88162	3.10%	0.360%
25	14.568	2118	2122	2129	rBV	96007	99802	3.50%	0.407%
26	14.886	2171	2176	2182	rBV	149314	163307	5.73%	0.666%
27	15.233	2231	2235	2246	rVB	178723	228153	8.01%	0.931%
28	15.633	2298	2303	2304	rBV	214192	248302	8.72%	1.013%
29	15.656	2304	2307	2318	rVB	331049	469885	16.50%	1.918%
30	16.086	2375	2380	2386	rBV	135292	216561	7.60%	0.884%
31	16.162	2388	2393	2398	rBV7	30389	56608	1.99%	0.231%
32	16.621	2465	2471	2478	rVB	75357	137358	4.82%	0.561%
33	17.245	2572	2577	2583	rVB2	28934	55878	1.96%	0.228%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

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-BF102318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

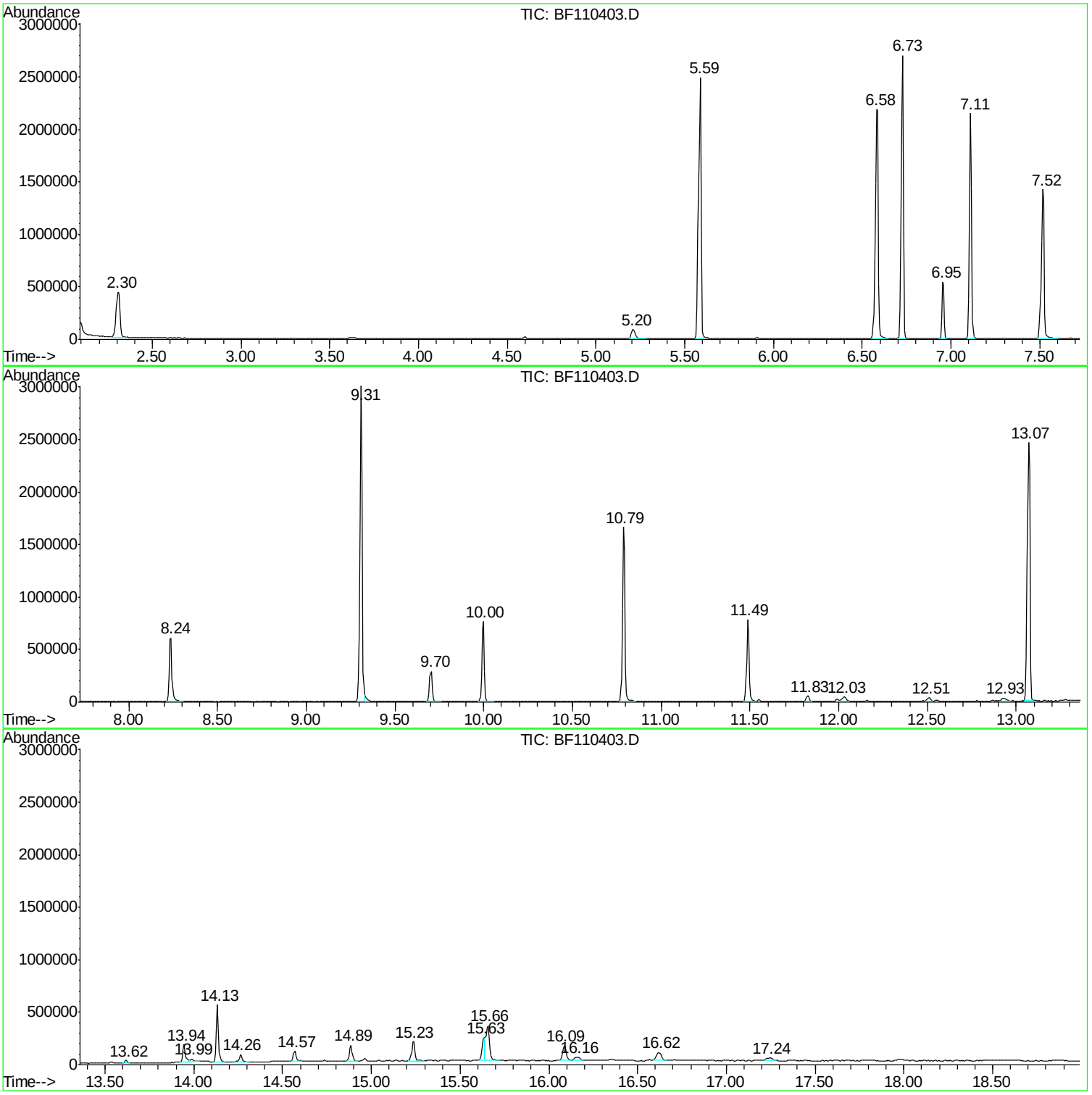
Sum of corrected areas: 24504461

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

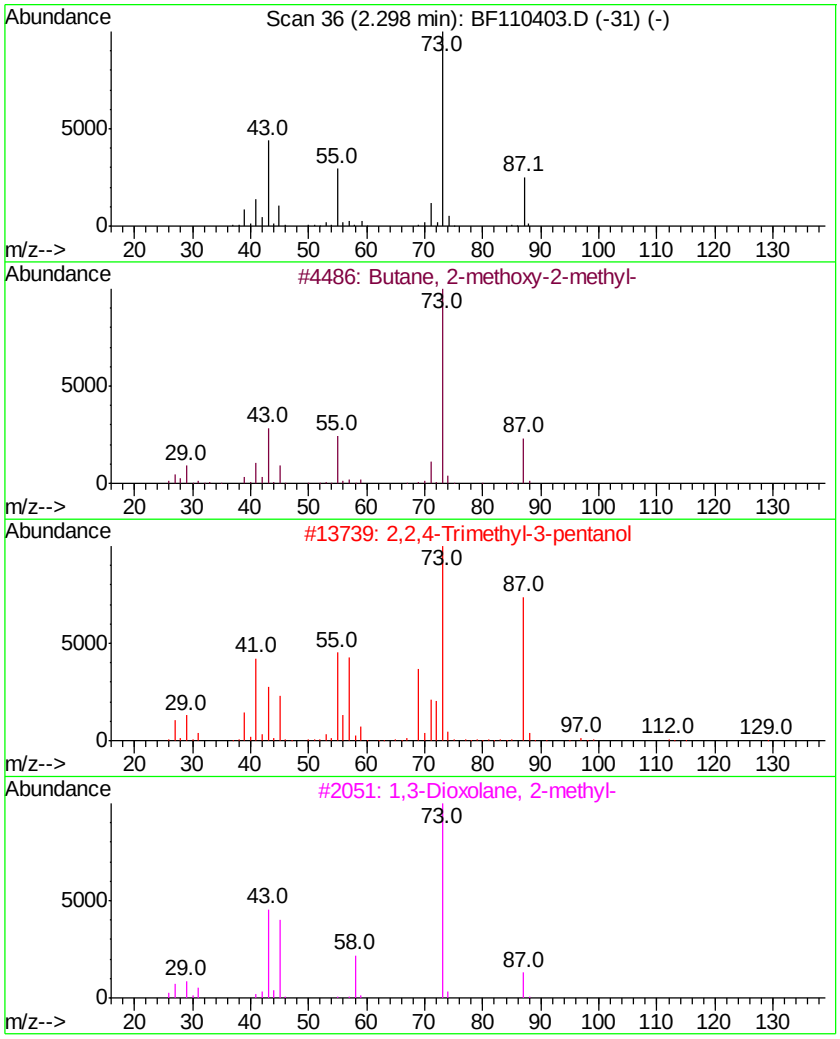
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

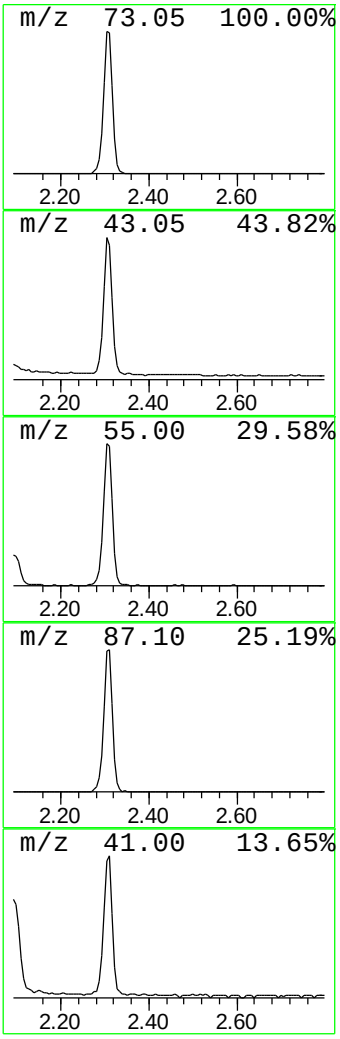
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	24.20 ng	603242	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

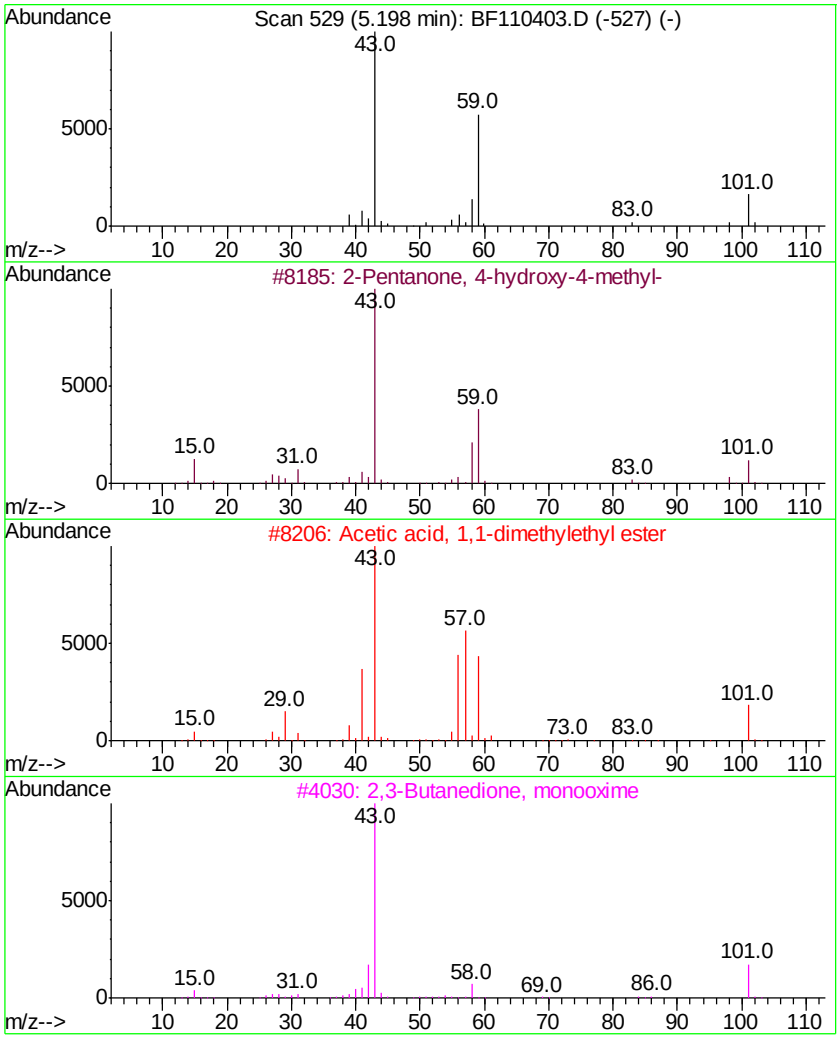
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

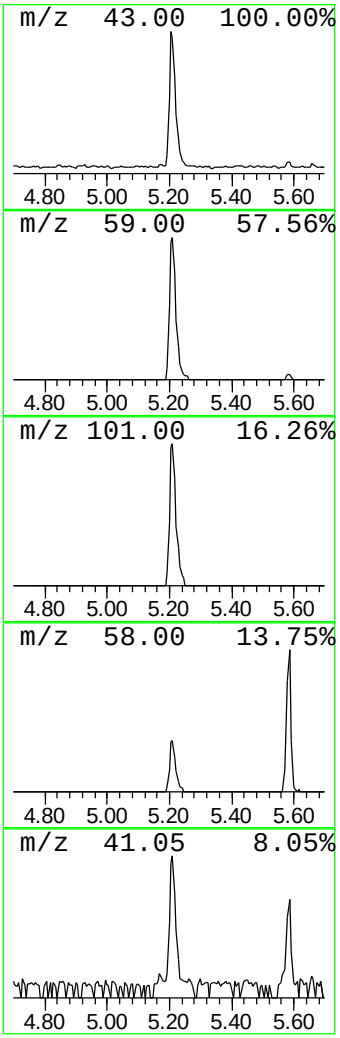
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	5.20 ng	129720	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4	Guanidine	59	CH5N3	000113-00-8	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

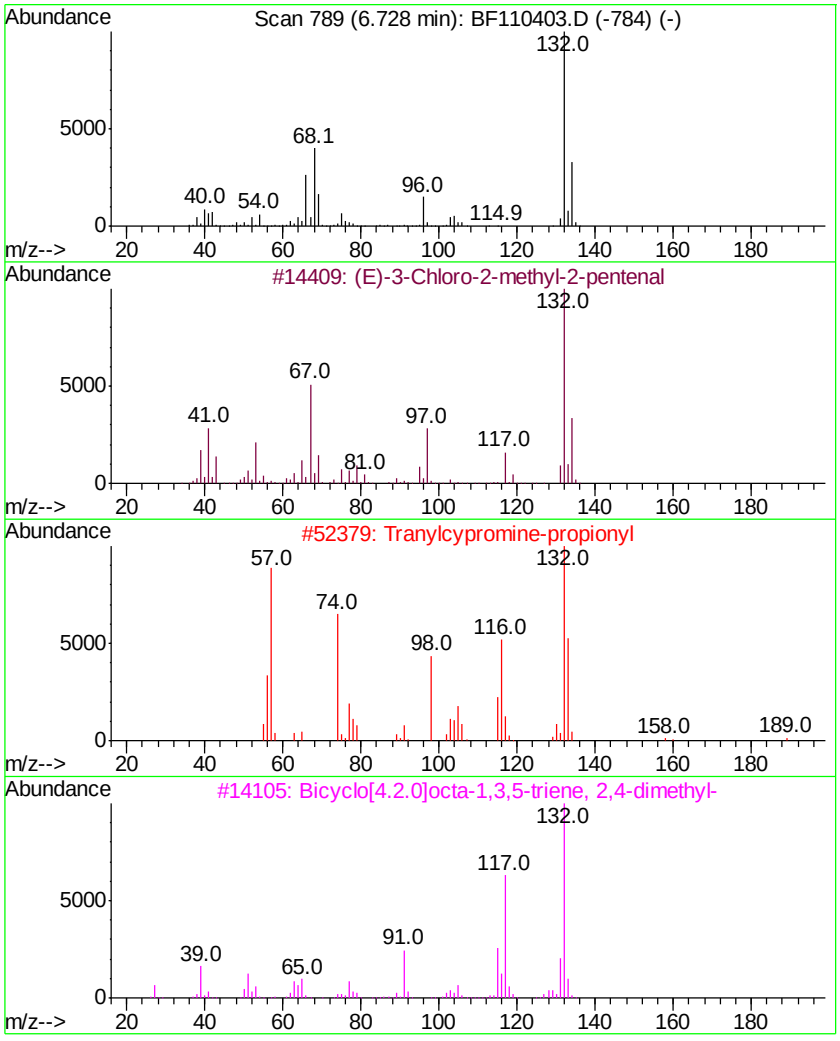
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

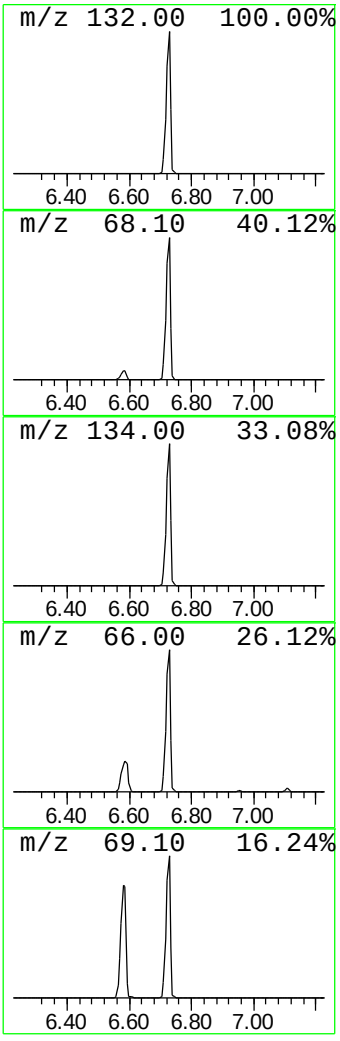
****

Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	104.24 ng	2598290	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

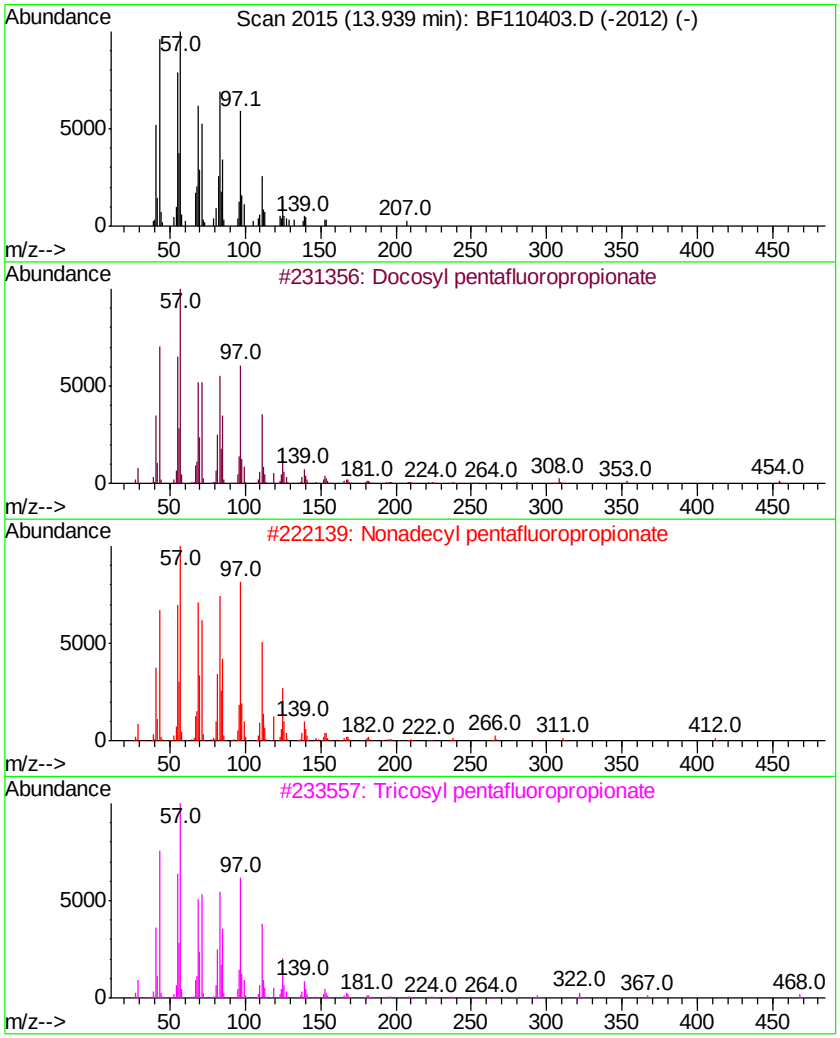
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

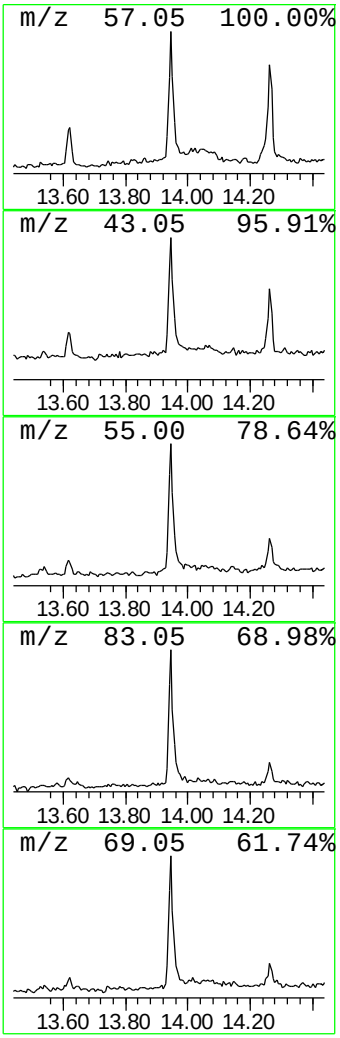
****

Peak Number 5 Docosyl pentafluoropropionate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	7.09 ng	176454	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

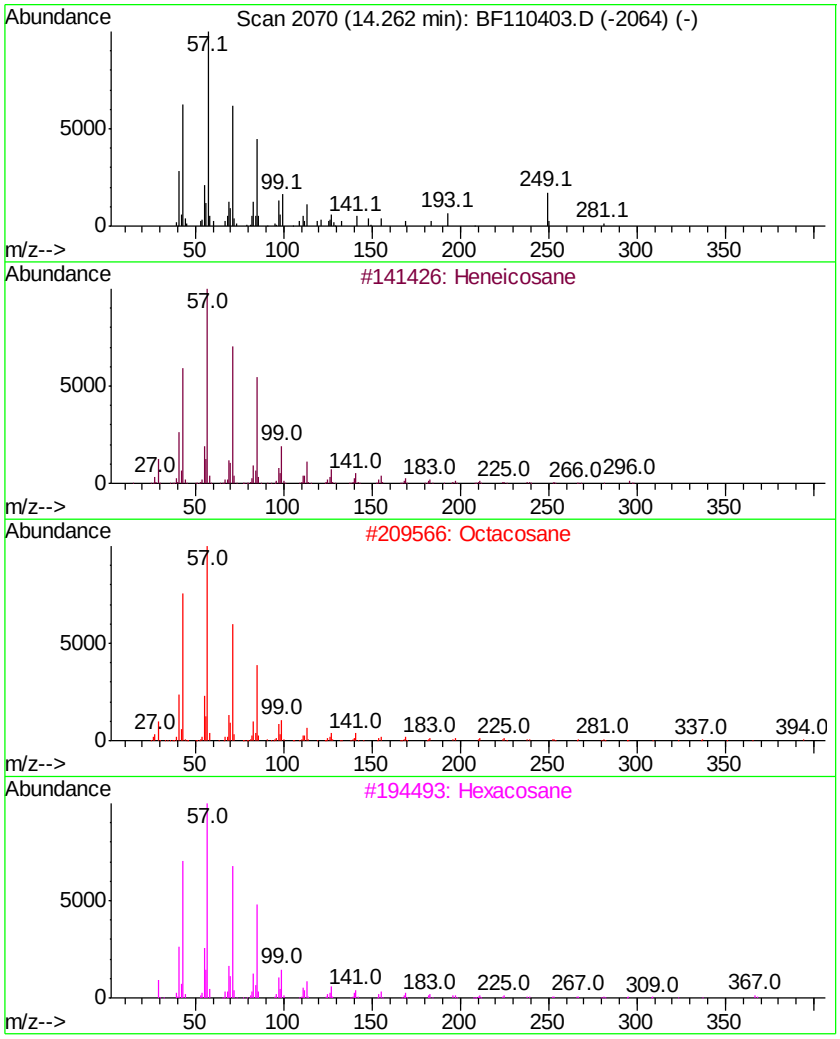
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

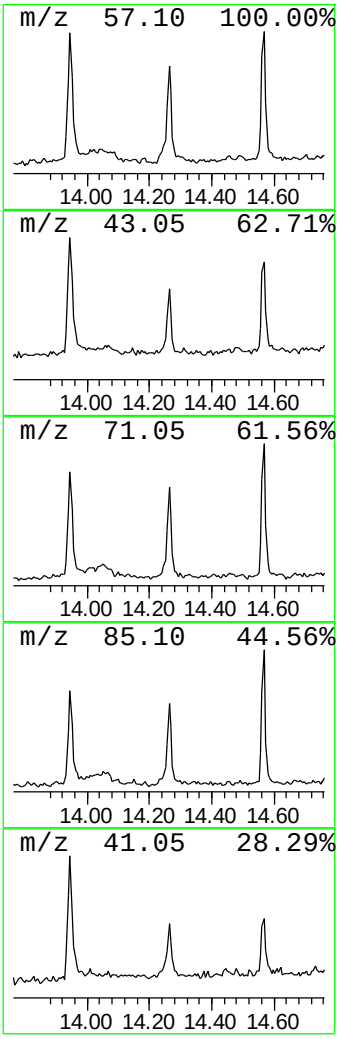
****

Peak Number 6 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	3.54 ng	88162	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Pentacosane	352	C25H52	000629-99-2	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

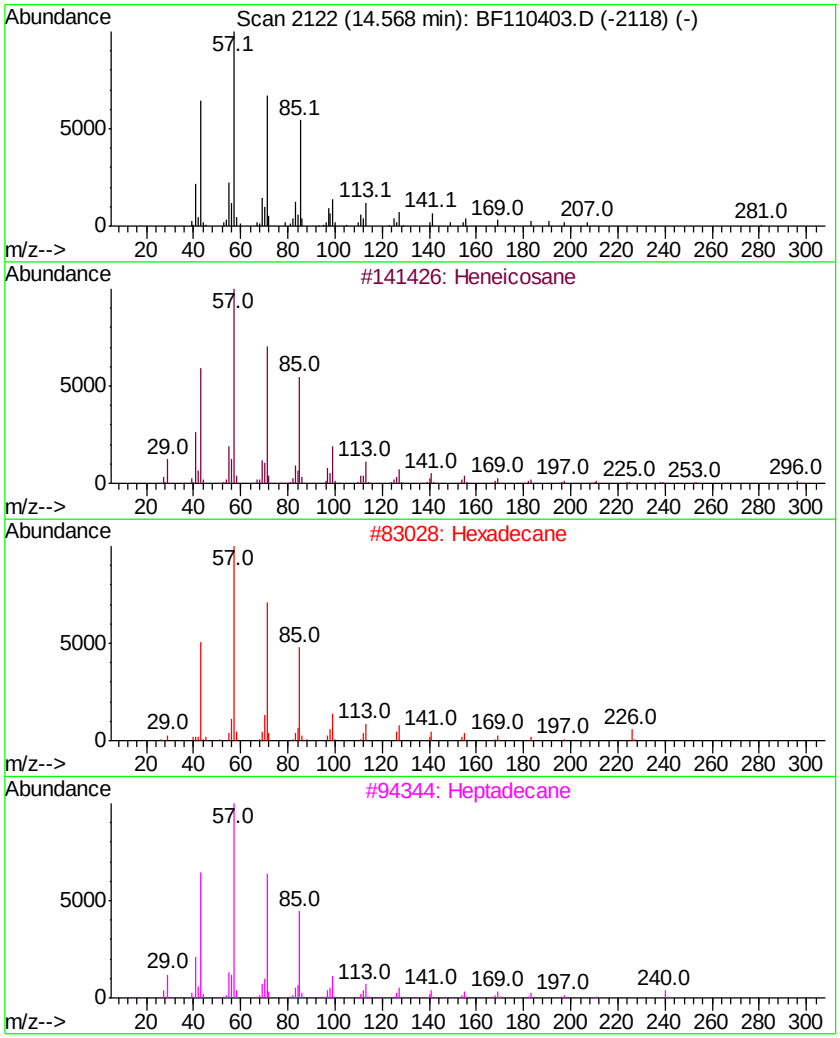
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

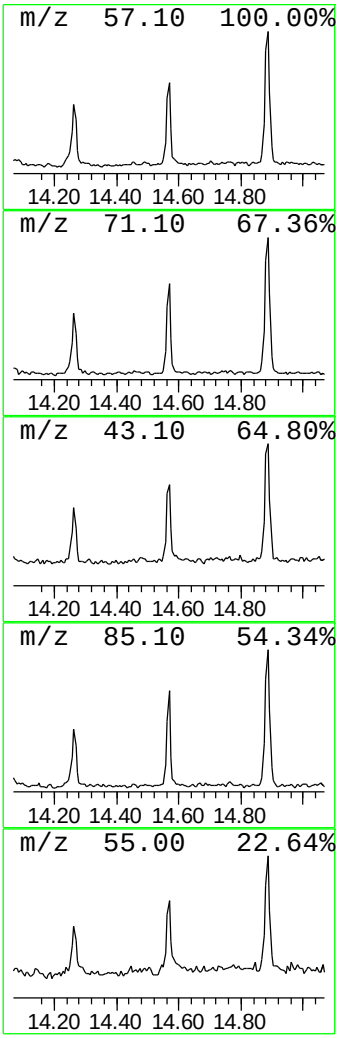
****

Peak Number 7 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	4.01 ng	99802	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

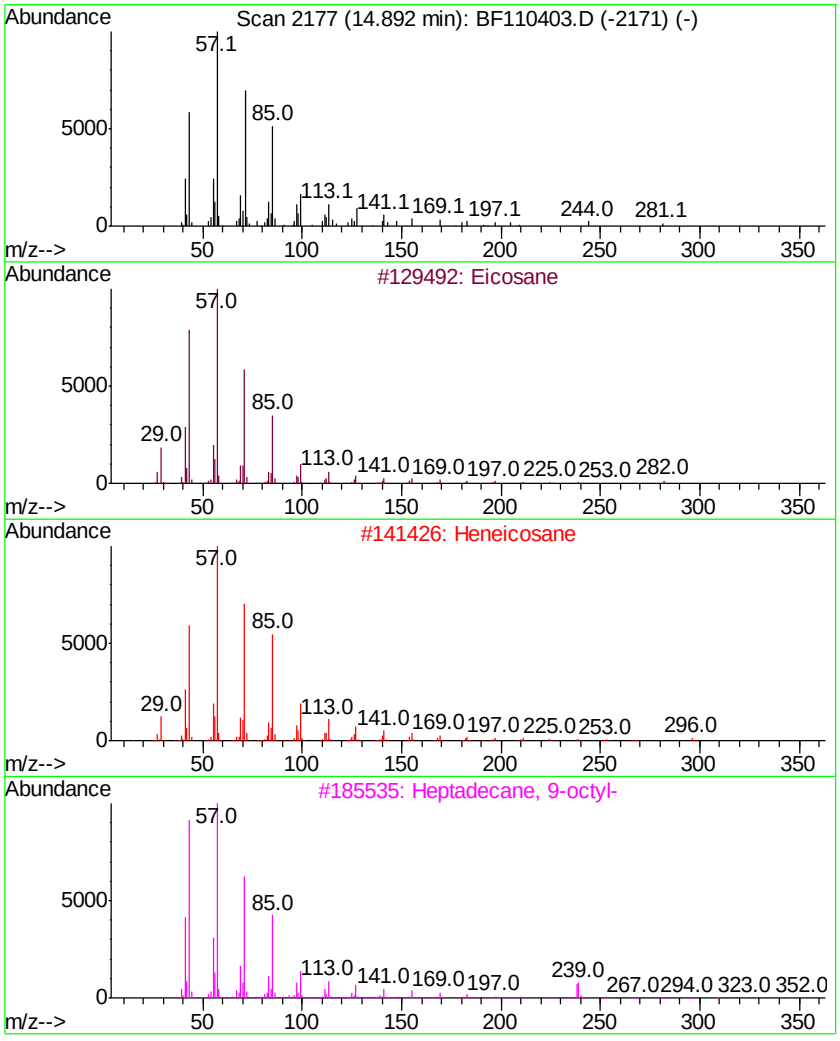
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

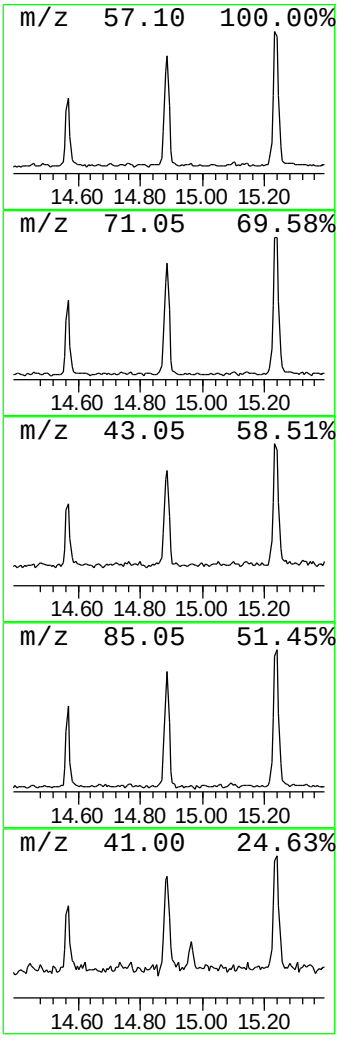
****

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	6.56 ng	163307	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Docosane	310	C22H46	000629-97-0	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

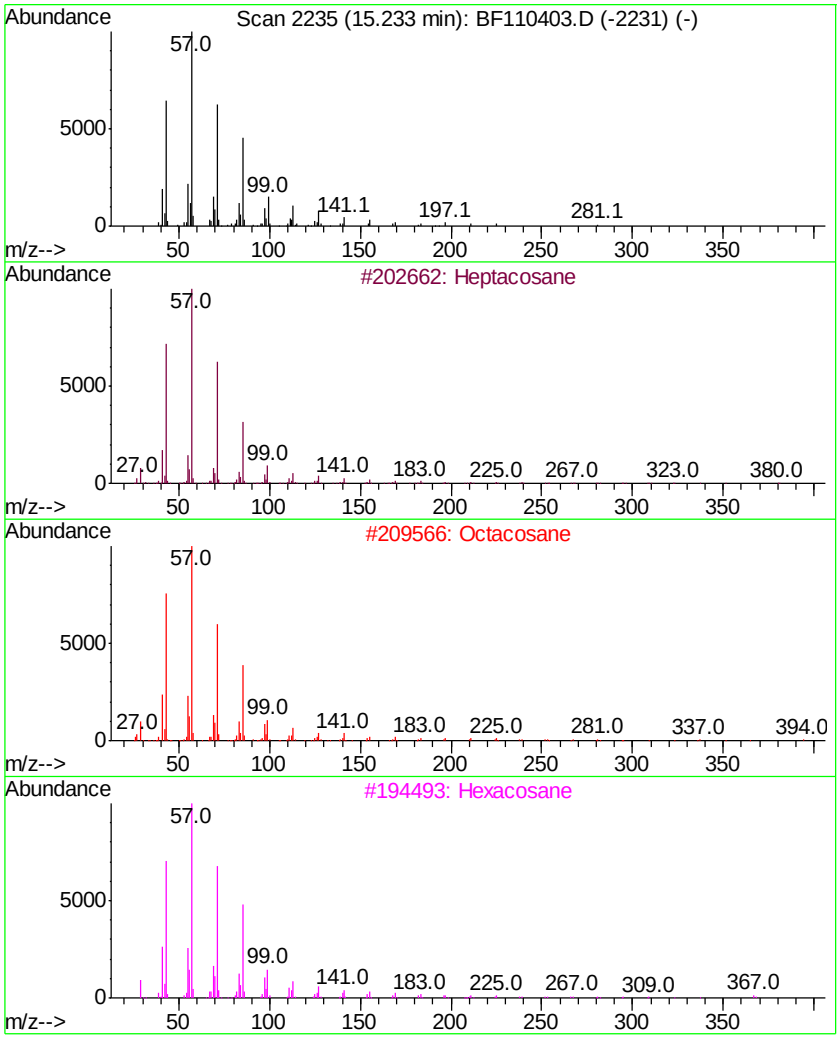
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

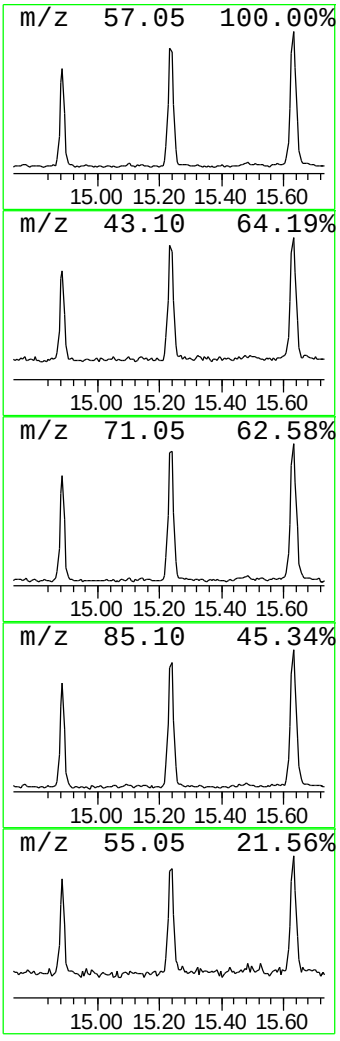
****

Peak Number 9 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	9.71 ng	228153	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

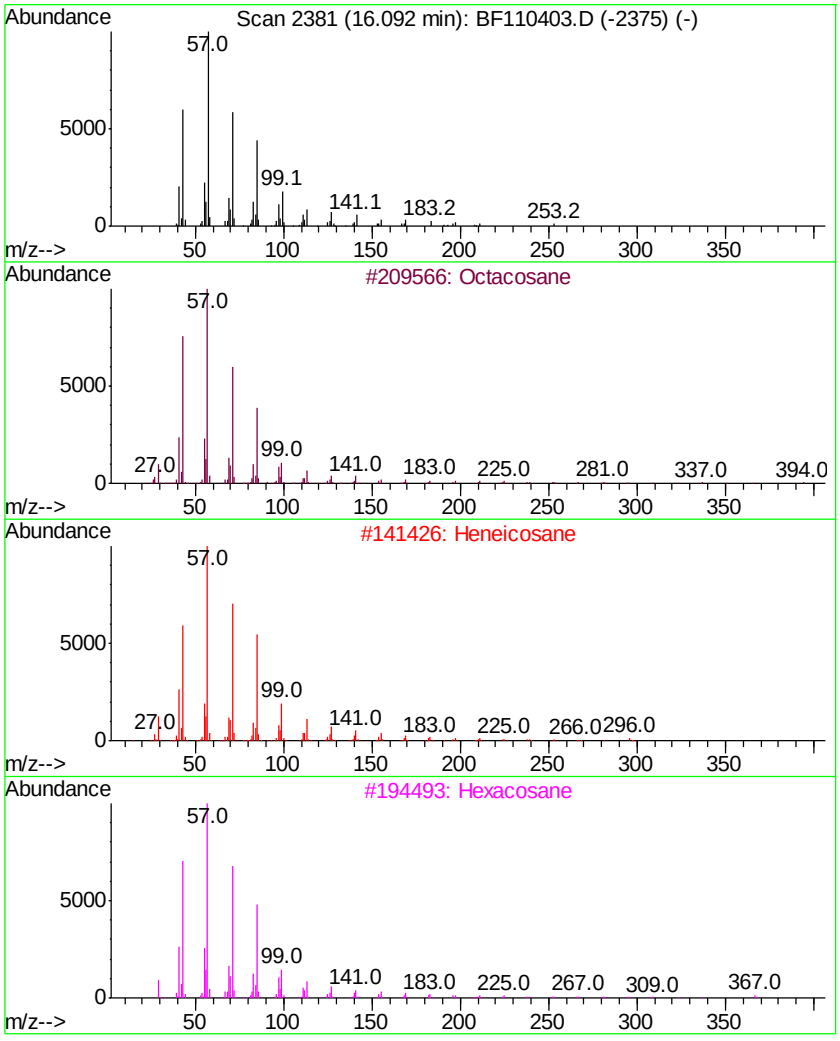
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

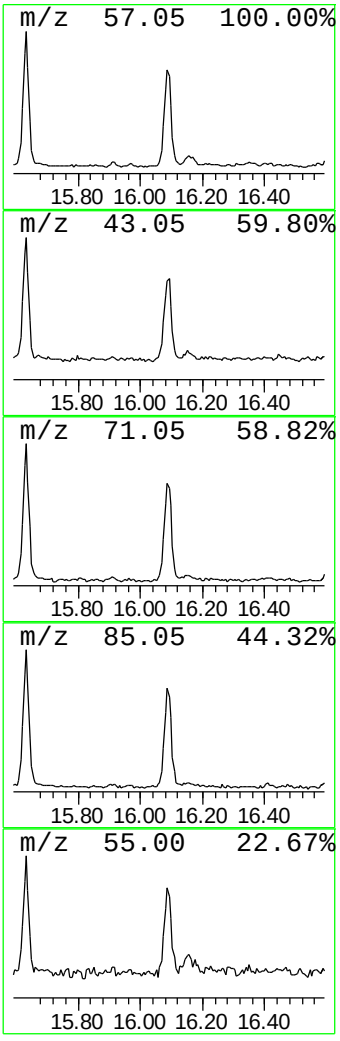
****

Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	9.22 ng	216561	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

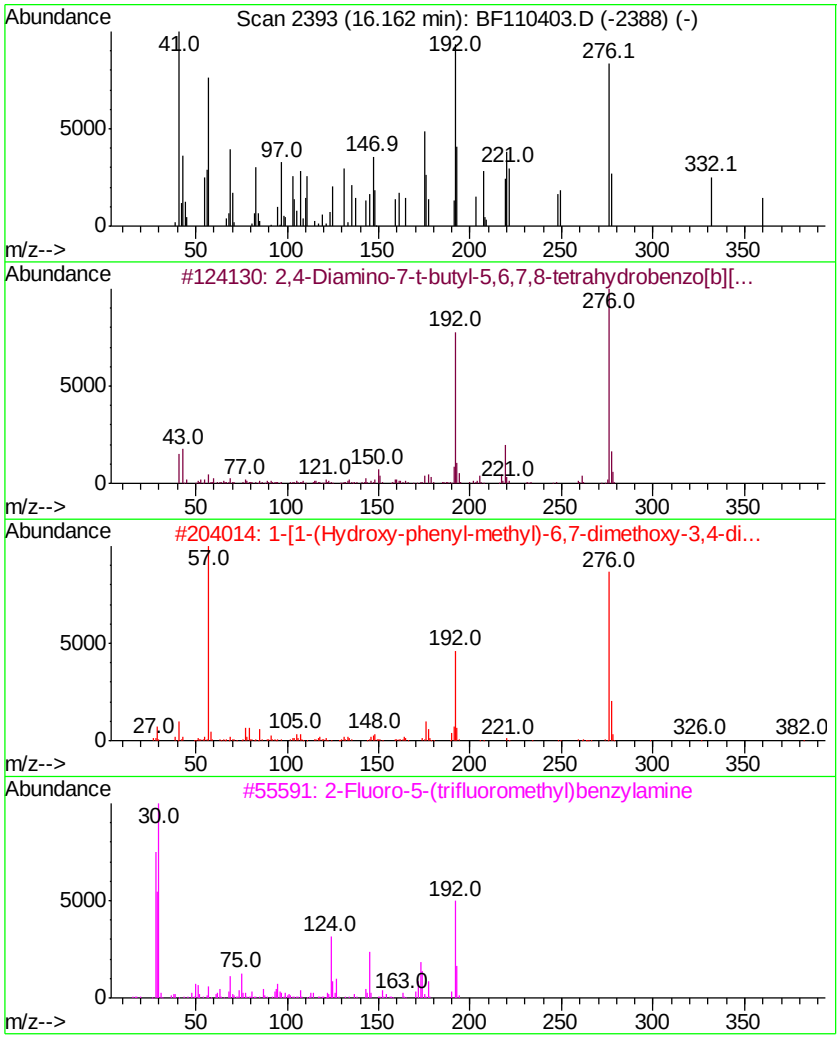
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

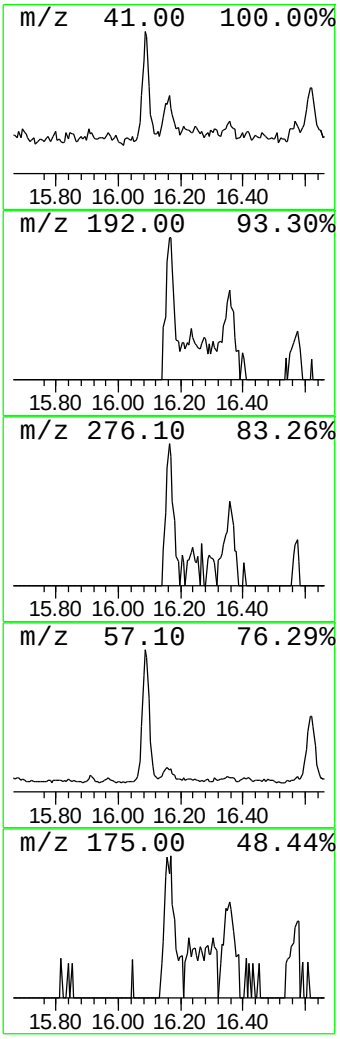
****

Peak Number 11 unknown16.16 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	2.41 ng	56608	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Diamino-7-t-butyl-5,6,7,8-te...	276	C14H20N4S	049620-43-1	43
2	1-[1-(Hydroxy-phenyl-methyl)-6,7...	383	C23H29NO4	114609-12-0	37
3	2-Fluoro-5-(trifluoromethyl)benz...	193	C8H7F4N	199296-61-2	22
4	(E)-2-[1-(3-Hydroxy-2-furanyl)et...	192	C10H8O4	105399-03-9	22
5	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	14





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

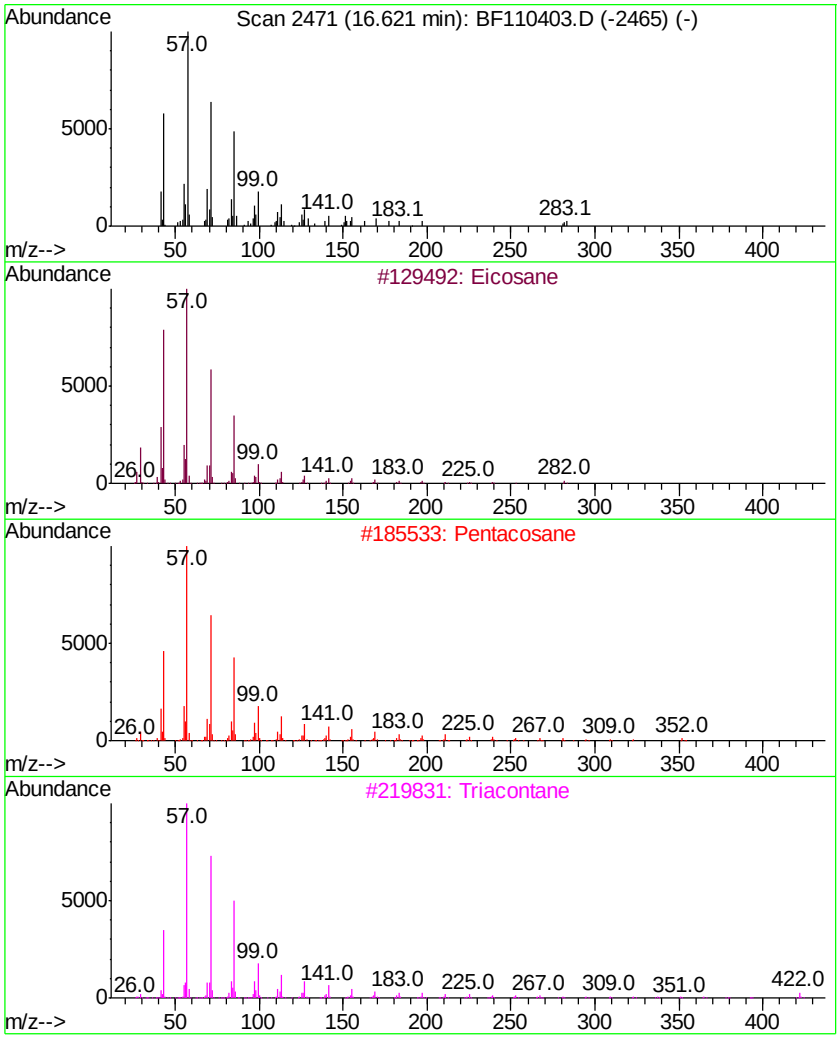
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

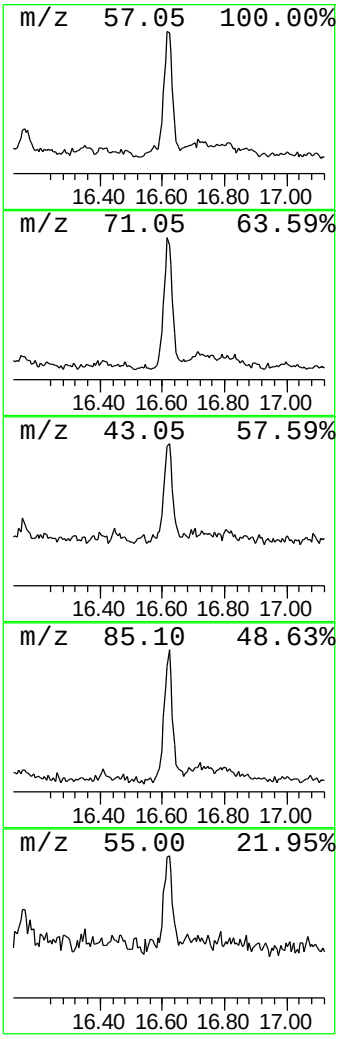
****

Peak Number 12 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	5.85 ng	137358	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Pentacosane	352	C25H52	000629-99-2	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Docosane	310	C22H46	000629-97-0	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

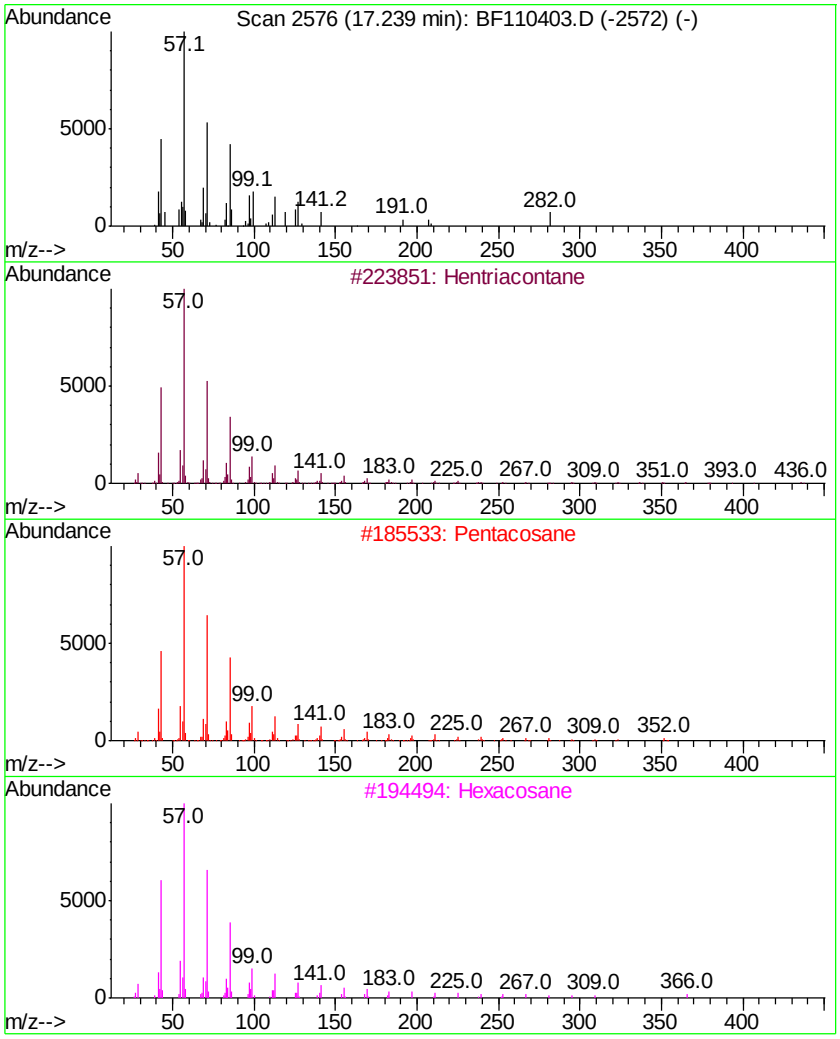
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

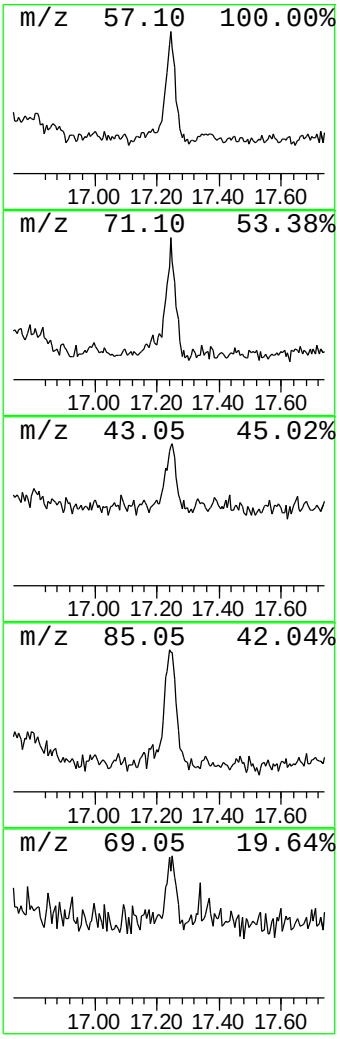
****

Peak Number 13 Hentriacontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.24	2.38 ng	55878	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	83
2	Pentacosane	352	C25H52	000629-99-2	83
3	Hexacosane	366	C26H54	000630-01-3	83
4	Octacosane	394	C28H58	000630-02-4	80
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110218\
Data File : BF110403.D
Acq On : 2 Nov 2018 11:14
Operator : JU/SJ
Sample : J5741-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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
Butane, 2-methoxy...	2.30	24.2	ng	603242	1	6.96	498522	20.0
2-Pentanone, 4-hy...	5.20	5.2	ng	129720	1	6.96	498522	20.0
unknown6.73	6.73	104.2	ng	2598290	1	6.96	498522	20.0
Docosyl pentafluo...	13.94	7.1	ng	176454	5	14.13	497897	20.0
Hexacosane	14.26	3.5	ng	88162	5	14.13	497897	20.0
Heneicosane	14.57	4.0	ng	99802	5	14.13	497897	20.0
Eicosane	14.89	6.6	ng	163307	5	14.13	497897	20.0
Heptacosane	15.23	9.7	ng	228153	6	15.66	469885	20.0
Octacosane	16.09	9.2	ng	216561	6	15.66	469885	20.0
unknown16.16	16.16	2.4	ng	56608	6	15.66	469885	20.0
Pentacosane	16.62	5.8	ng	137358	6	15.66	469885	20.0
Hentriacontane	17.24	2.4	ng	55878	6	15.66	469885	20.0