LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110518\
Data File : BF110466.D
Acq On : 5 Nov 2018 15:49
Operator : JU/SJ
Sample : J5812-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-A

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	2.316	31	39	48	rBV	382711	503611	18.86%	2.307%
2	5.204	526	530	538	rBV	58365	81736	3.06%	0.374%
3	5.581	590	594	597	rBV	2115124	1963102	73.53%	8.993%
4	6.581	759	764	784	rBV	2054910	2295212	85.97%	10.514%
5	6.722	784	788	792	rBV	2178521	2220860	83.18%	10.174%
6	6.951	824	827	833	rBV	634611	556751	20.85%	2.550%
7	7.110	849	854	868	rBV	1845553	1687293	63.20%	7.729%
8	7.516	918	923	938	rBV	1245350	1417060	53.08%	6.492%
9	8.239	1041	1046	1064	rBV	666447	774706	29.02%	3.549%
10	9.310	1222	1228	1238	rBV	2821422	2669806	100.00%	12.230%
11	9.704	1290	1295	1307	rBV	299761	327678	12.27%	1.501%
12	9.998	1339	1345	1358	rBV	952612	928226	34.77%	4.252%
13	10.786	1475	1479	1492	rBV	1572810	1596851	59.81%	7.315%
14	11.486	1594	1598	1606	rBV	837427	926628	34.71%	4.245%
15	13.068	1863	1867	1871	rBV	2395137	2267554	84.93%	10.388%
16	13.951	2011	2017	2027	rBV2	67405	128601	4.82%	0.589%
17	14.133	2044	2048	2058	rBV	544179	571011	21.39%	2.616%
18	14.262	2064	2070	2076	rBV	21775	28701	1.08%	0.131%
19	14.562	2116	2121	2125	rBV	34668	36760	1.38%	0.168%
20	14.880	2171	2175	2180	rBV	51154	53644	2.01%	0.246%
21	15.233	2228	2235	2243	rBV	66897	85279	3.19%	0.391%
22	15.627	2298	2302	2304	rBV	65962	85817	3.21%	0.393%
23	15.662	2304	2308	2318	rVB	267460	413419	15.48%	1.894%
24	16.080	2375	2379	2388	rVB	63212	101040	3.78%	0.463%
25	16.615	2464	2470	2475	rBV2	38869	73414	2.75%	0.336%
26	17.239	2571	2576	2581	rVB5	17499	34618	1.30%	0.159%

Sum of corrected areas: 21829378

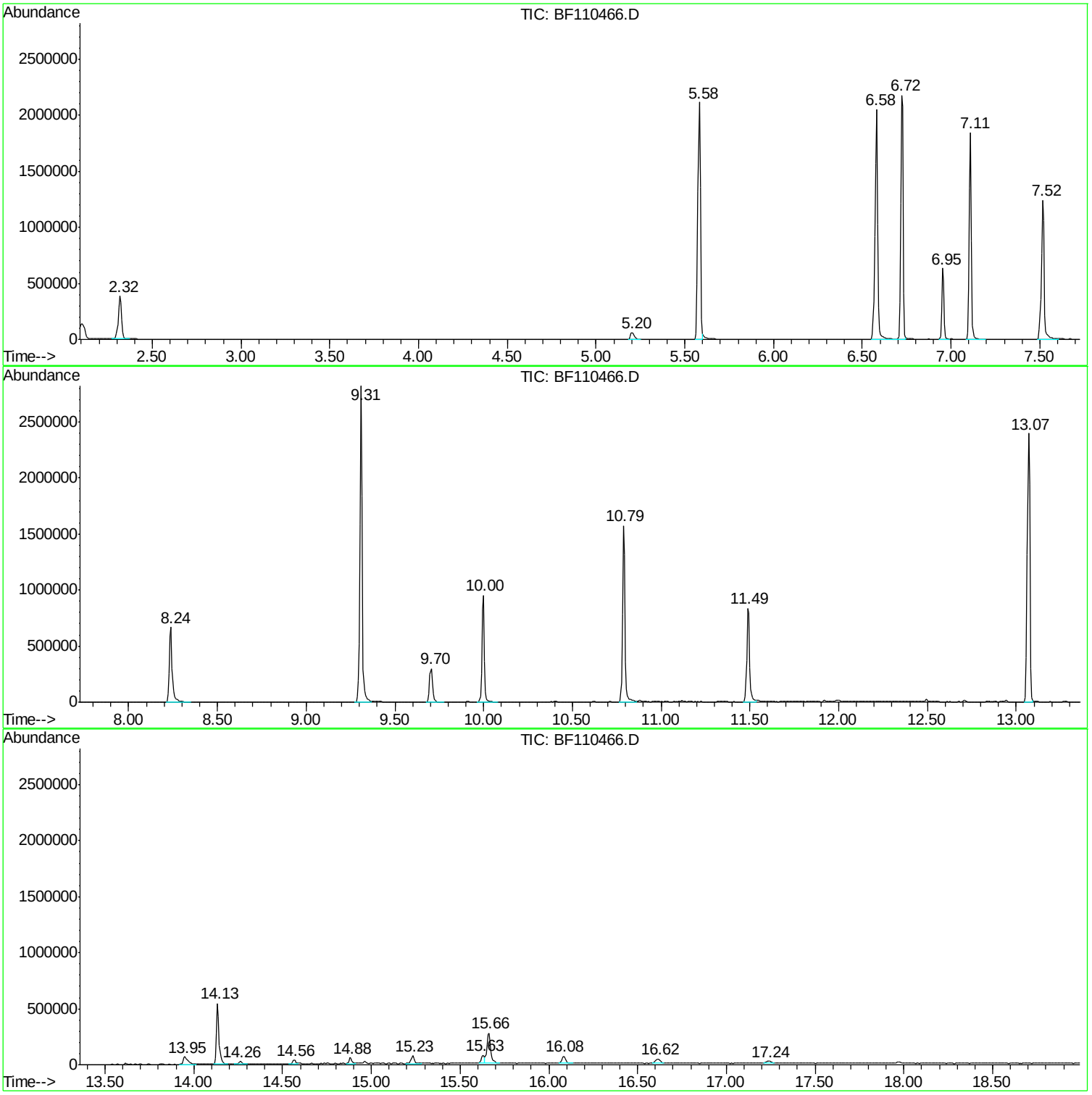
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110518\
Data File : BF110466.D
Acq On : 5 Nov 2018 15:49
Operator : JU/SJ
Sample : J5812-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-A

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110518\
Data File : BF110466.D
Acq On : 5 Nov 2018 15:49
Operator : JU/SJ
Sample : J5812-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-A

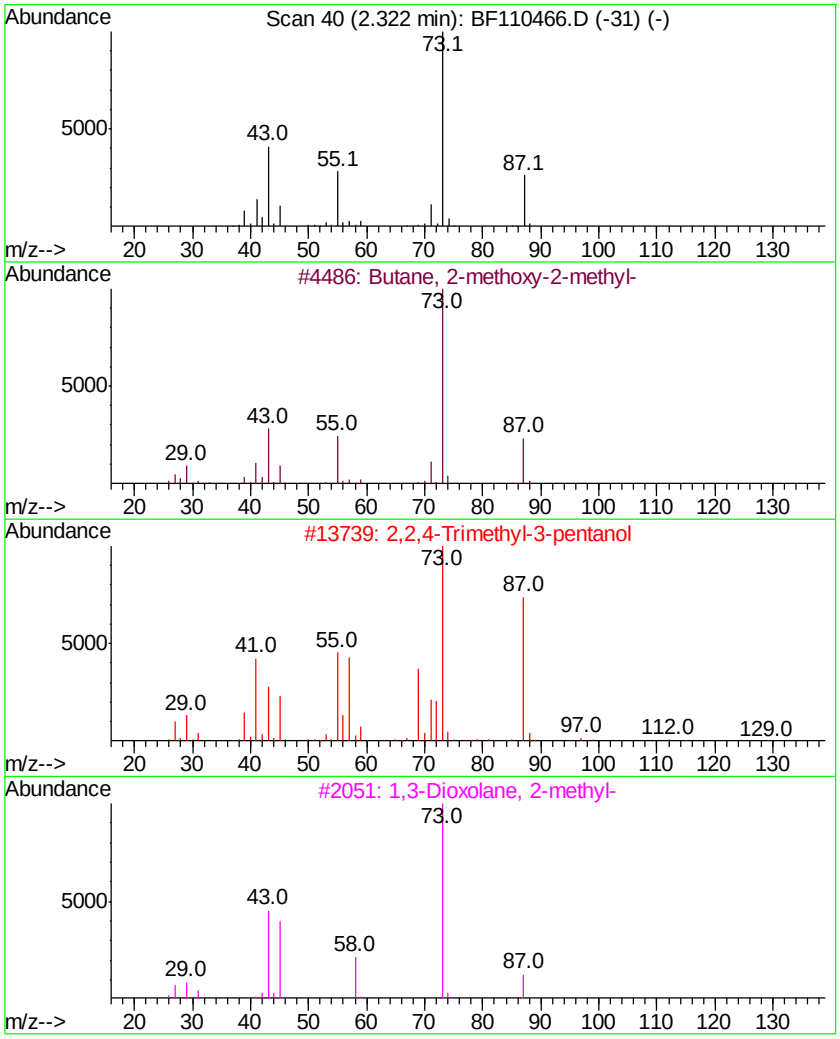
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

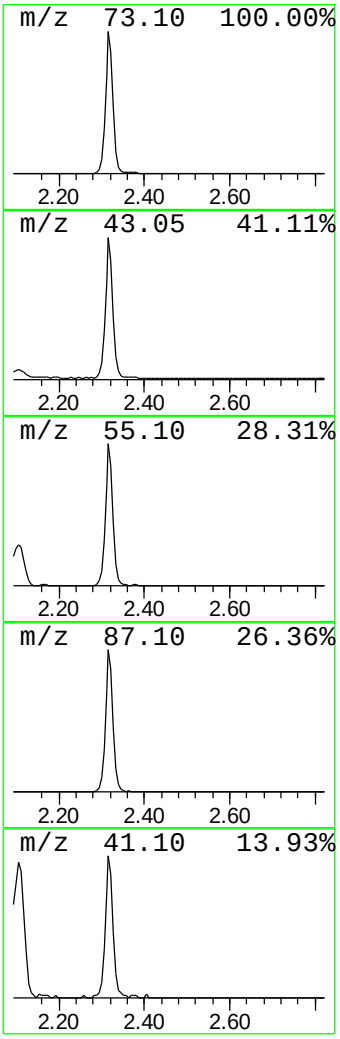
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	18.09 ng	503611	1,4-Dichlorobenzene-d4	6.95

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	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

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Data File : BF110466.D
Acq On : 5 Nov 2018 15:49
Operator : JU/SJ
Sample : J5812-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-A

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

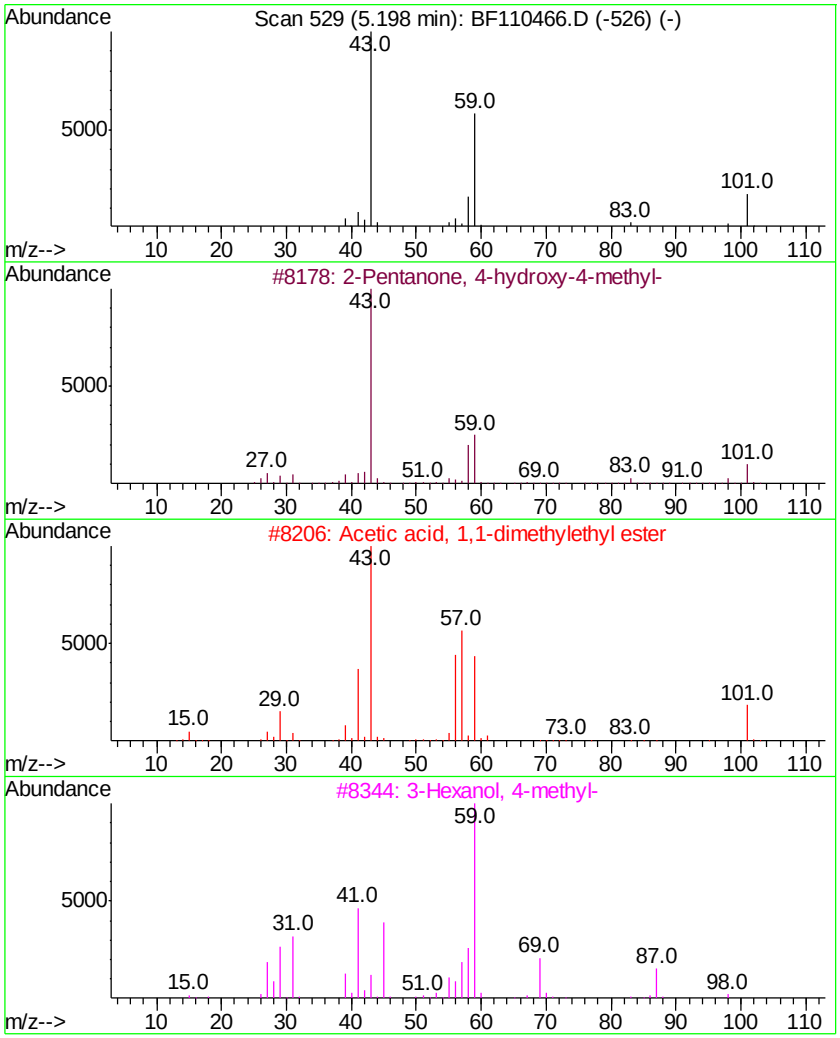
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

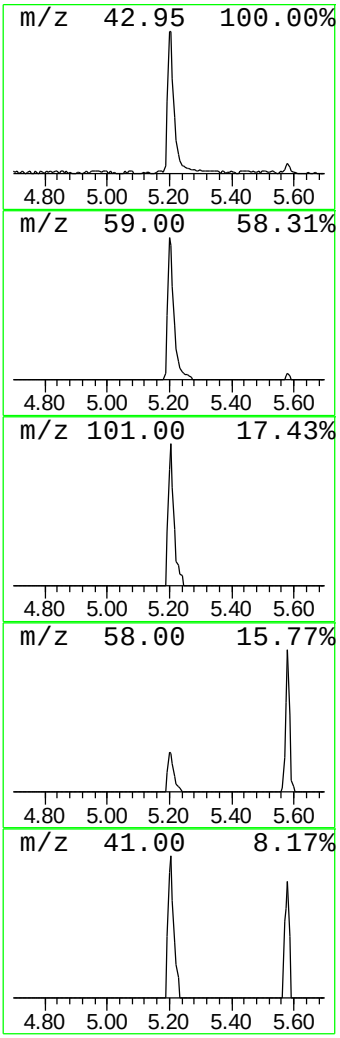
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.94 ng	81736	1,4-Dichlorobenzene-d4	6.95

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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110518\
Data File : BF110466.D
Acq On : 5 Nov 2018 15:49
Operator : JU/SJ
Sample : J5812-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-A

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

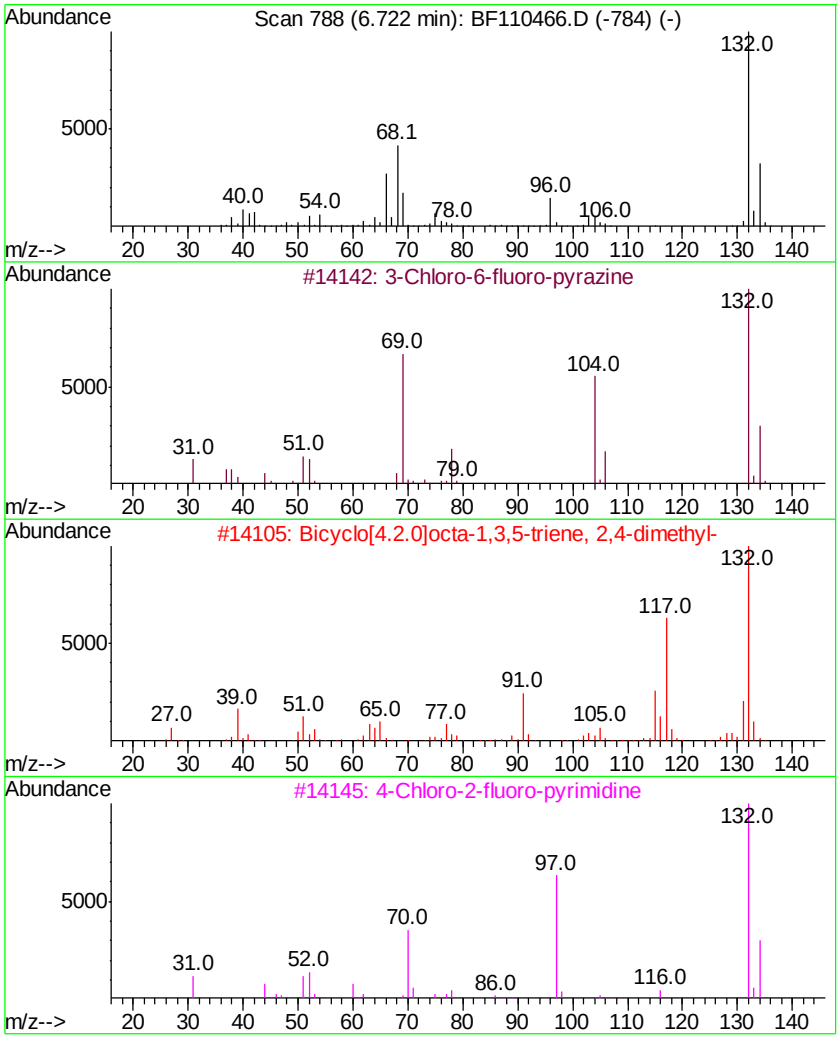
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

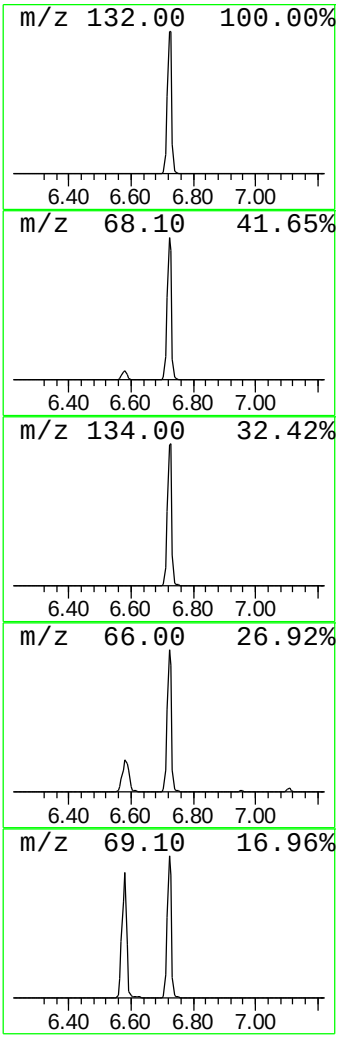
****

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	79.78 ng	2220860	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110518\
Data File : BF110466.D
Acq On : 5 Nov 2018 15:49
Operator : JU/SJ
Sample : J5812-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-A

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

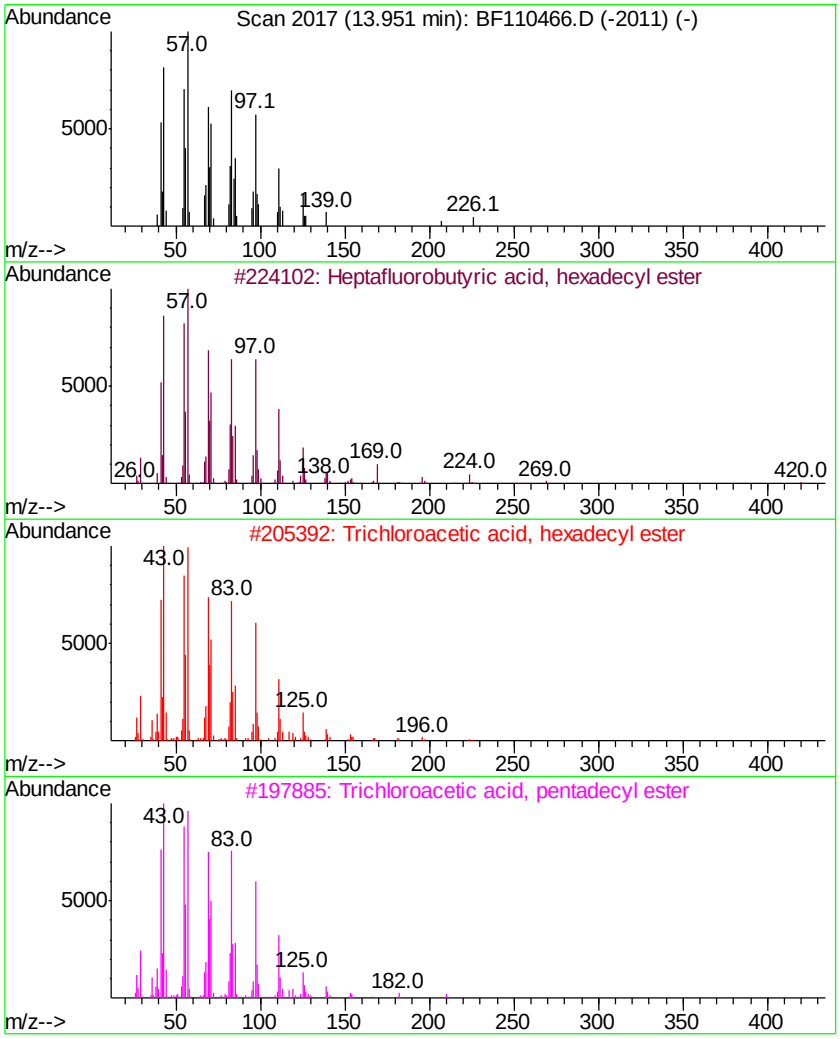
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

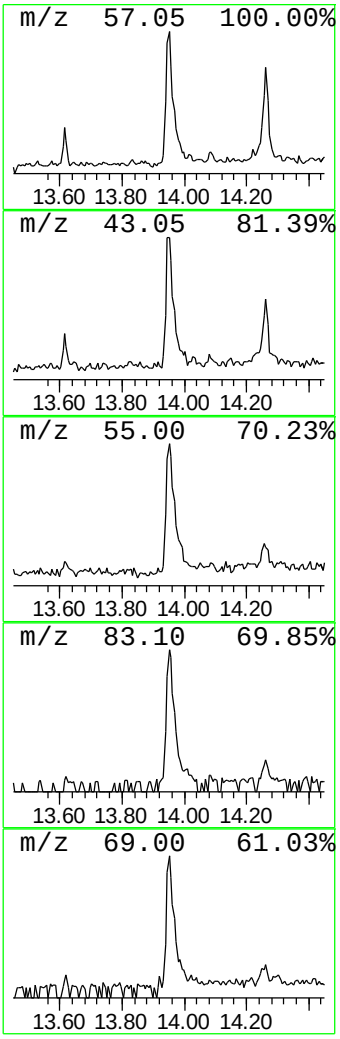
****

Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.50 ng	128601	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110518\
Data File : BF110466.D
Acq On : 5 Nov 2018 15:49
Operator : JU/SJ
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-A

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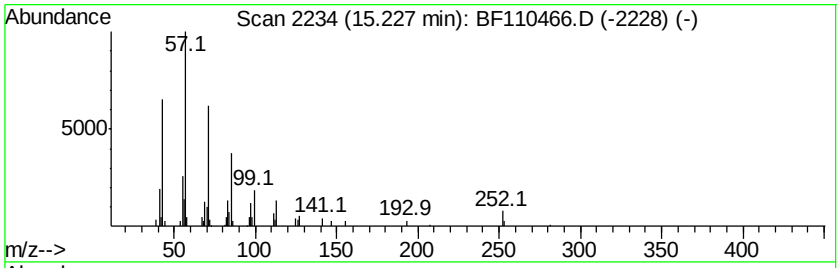
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

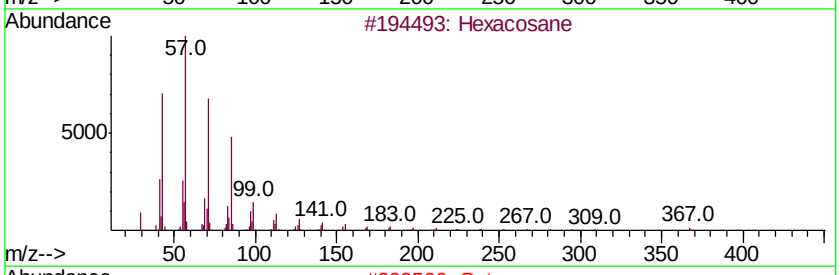
****

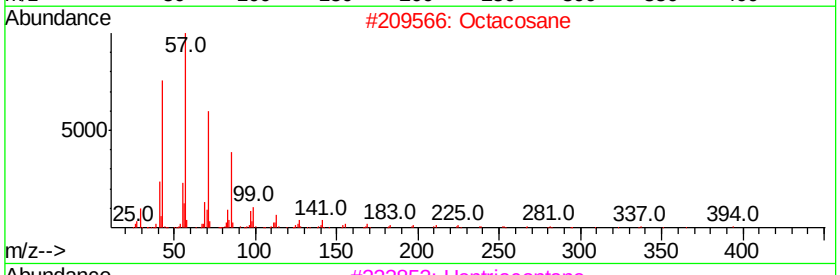
Peak Number 6 Hexacosane Concentration Rank 6

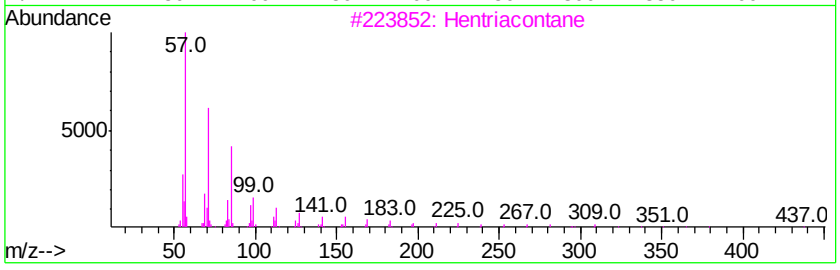
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	4.13 ng	85279	Perylene-d12	15.66

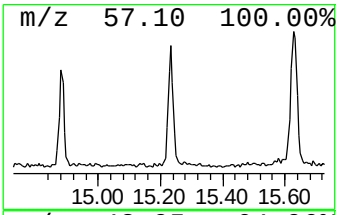
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Heptacosane	380	C27H56	000593-49-7	87
5	Hexadecane	226	C16H34	000544-76-3	87

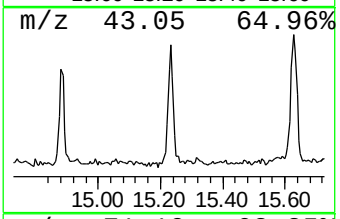


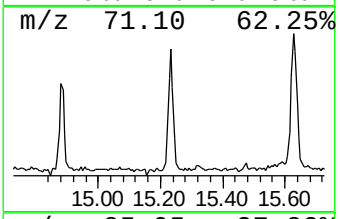


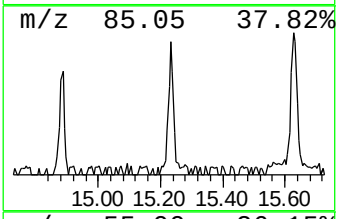


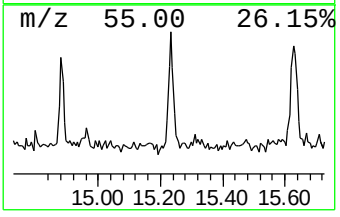












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110518\
Data File : BF110466.D
Acq On : 5 Nov 2018 15:49
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-A

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

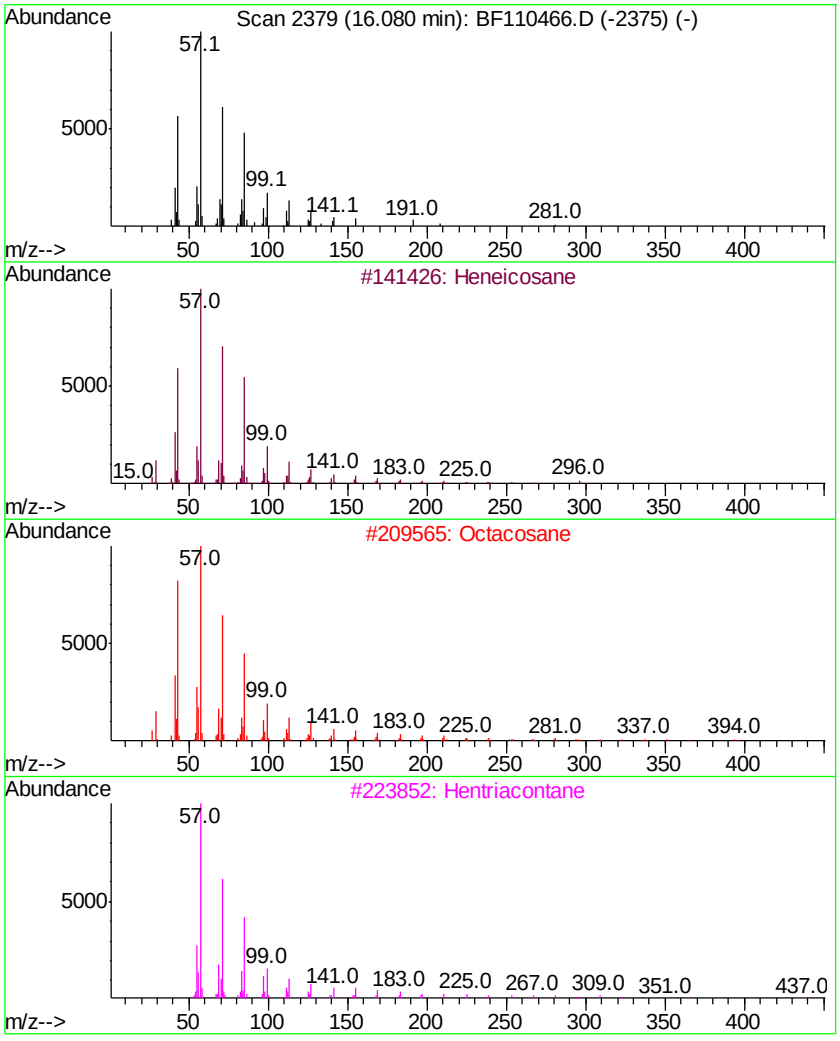
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

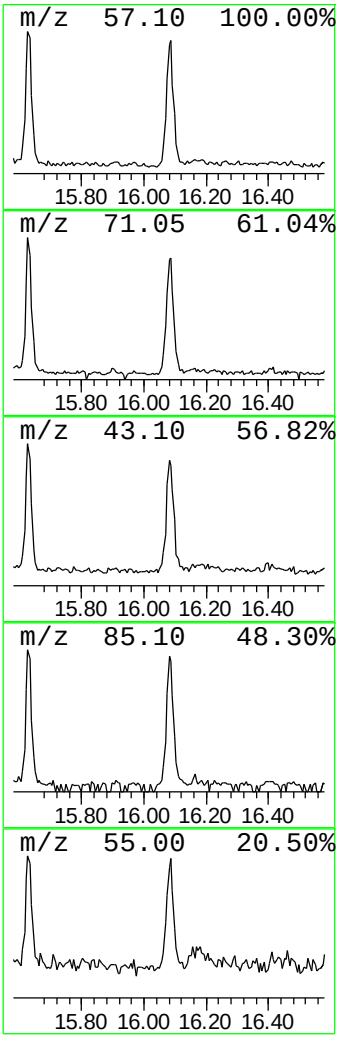
****

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	4.89 ng	101040	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Triacontane	422	C30H62	000638-68-6	90
5	Hexacosane	366	C26H54	000630-01-3	87





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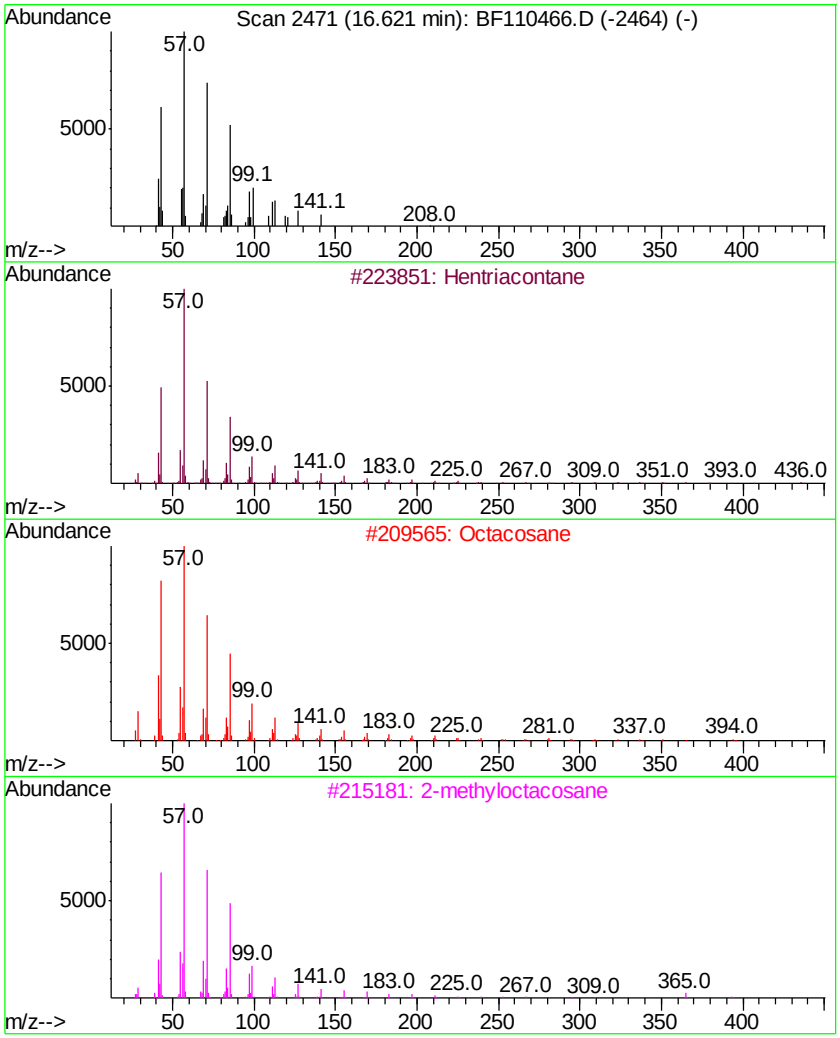
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

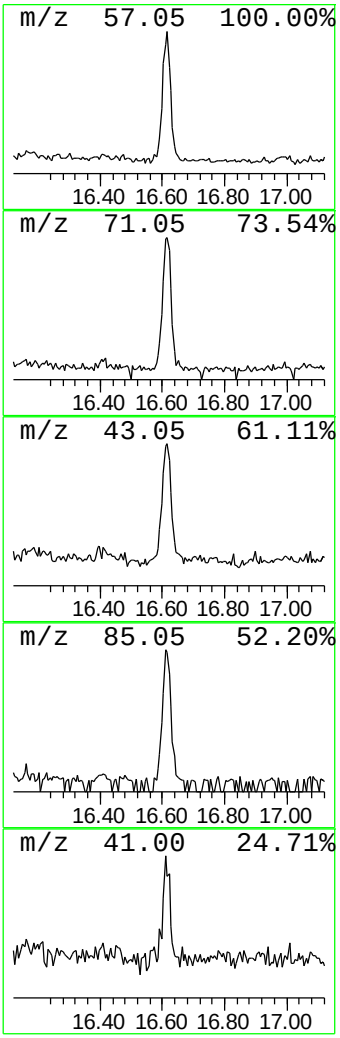
****

Peak Number 8 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	3.55 ng	73414	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	87
2	Octacosane	394	C28H58	000630-02-4	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	86
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Hexacosane	366	C26H54	000630-01-3	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110518\
Data File : BF110466.D
Acq On : 5 Nov 2018 15:49
Operator : JU/SJ
Sample : J5812-09
Misc :
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Instrument : BNA_F
ClientSampleId : TP2-A

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...	2.32	18.1	ng	503611	1	6.95	556751	20.0
2-Pentanone, 4-hy...	5.20	2.9	ng	81736	1	6.95	556751	20.0
unknown6.72	6.72	79.8	ng	2220860	1	6.95	556751	20.0
Heptafluorobutyri...	13.95	4.5	ng	128601	5	14.13	571011	20.0
Hexacosane	15.23	4.1	ng	85279	6	15.66	413419	20.0
Heneicosane	16.08	4.9	ng	101040	6	15.66	413419	20.0
Hentriacontane	16.62	3.5	ng	73414	6	15.66	413419	20.0