LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110260.D
Acq On : 29 Oct 2018 14:12
Operator : JU/SJ
Sample : J5649-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DL-01A

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	2.310	33	38	49	rVB	255021	332080	13.54%	1.603%
2	5.204	527	530	542	rBV	71473	92101	3.76%	0.445%
3	5.592	591	596	599	rBV	2254637	2076964	84.71%	10.025%
4	6.592	760	766	778	rBV2	2098343	2414616	98.48%	11.655%
5	6.739	786	791	794	rBV	2317039	2243707	91.51%	10.830%
6	6.969	826	830	833	rBV	802796	660725	26.95%	3.189%
7	7.122	852	856	860	rBV	1925948	1739312	70.94%	8.396%
8	7.528	920	925	936	rBV	1373657	1400175	57.11%	6.759%
9	8.251	1044	1048	1054	rBV	937888	821714	33.52%	3.966%
10	9.322	1226	1230	1241	rBV	2518636	2451778	100.00%	11.835%
11	9.716	1293	1297	1305	rBV	278675	252859	10.31%	1.221%
12	10.010	1343	1347	1359	rVB2	967030	866693	35.35%	4.183%
13	10.804	1478	1482	1496	rBV	1215083	1165899	47.55%	5.628%
14	11.504	1597	1601	1610	rBV	804083	714969	29.16%	3.451%
15	12.010	1683	1687	1697	rBV4	30077	34084	1.39%	0.165%
16	13.086	1866	1870	1874	rBV	1831608	1627289	66.37%	7.855%
17	13.639	1959	1964	1971	rBV2	28431	34769	1.42%	0.168%
18	13.968	2016	2020	2031	rBV	97369	123719	5.05%	0.597%
19	14.151	2047	2051	2058	rBV	646833	595503	24.29%	2.874%
20	14.286	2071	2074	2079	rBV	56776	43859	1.79%	0.212%
21	14.592	2123	2126	2133	rBV	75663	88022	3.59%	0.425%
22	14.915	2177	2181	2186	rVB	76000	79382	3.24%	0.383%
23	15.268	2237	2241	2246	rVB	85407	91717	3.74%	0.443%
24	15.686	2305	2312	2321	rBV	382756	585219	23.87%	2.825%
25	16.133	2383	2388	2395	rBV2	62211	95175	3.88%	0.459%
26	16.674	2475	2480	2485	rVB2	30961	51794	2.11%	0.250%
27	17.303	2583	2587	2594	rVB6	15066	32993	1.35%	0.159%

Sum of corrected areas: 20717117

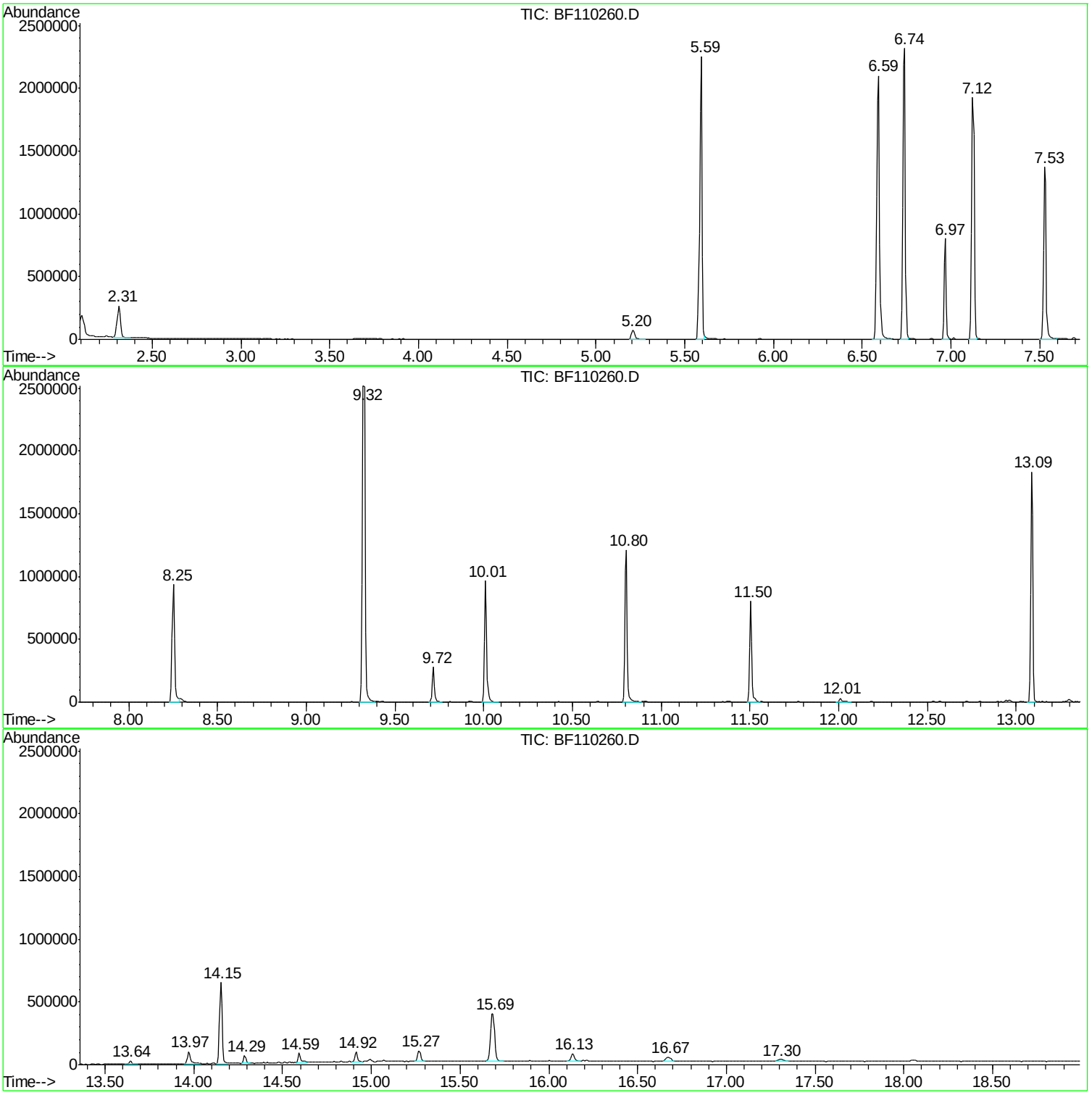
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110260.D
Acq On : 29 Oct 2018 14:12
Operator : JU/SJ
Sample : J5649-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DL-01A

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\BF102918\
Data File : BF110260.D
Acq On : 29 Oct 2018 14:12
Operator : JU/SJ
Sample : J5649-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DL-01A

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

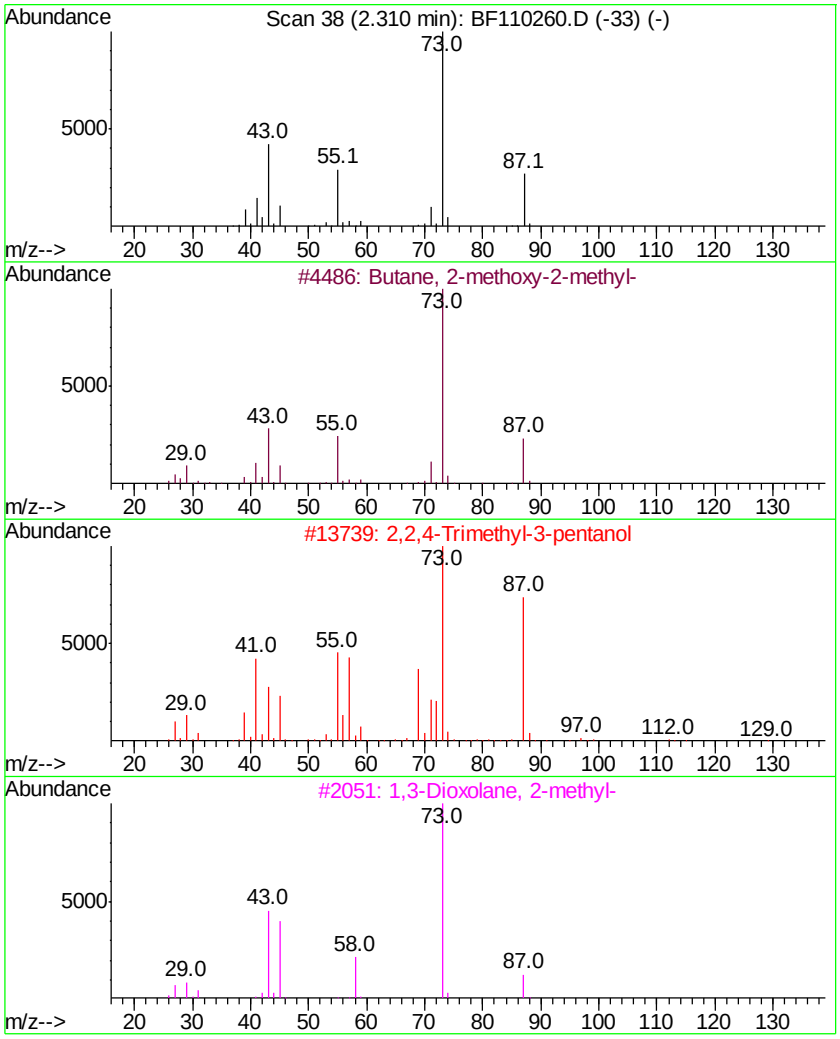
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

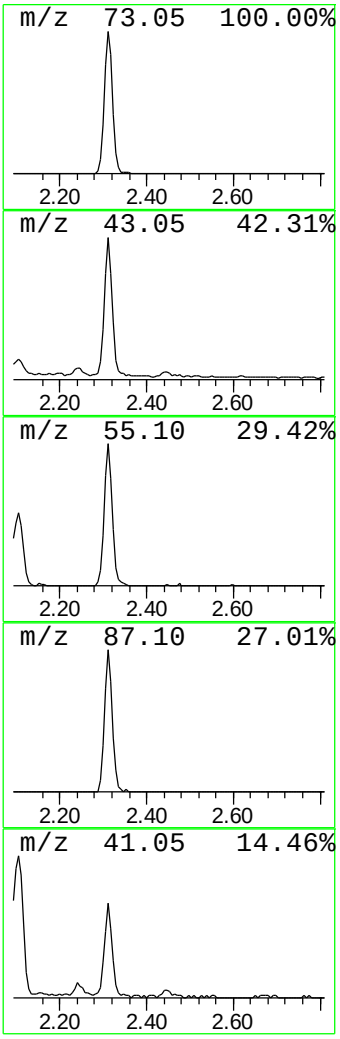
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	10.05 ng	332080	1,4-Dichlorobenzene-d4	6.97

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF110260.D
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Operator : JU/SJ
Sample : J5649-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DL-01A

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

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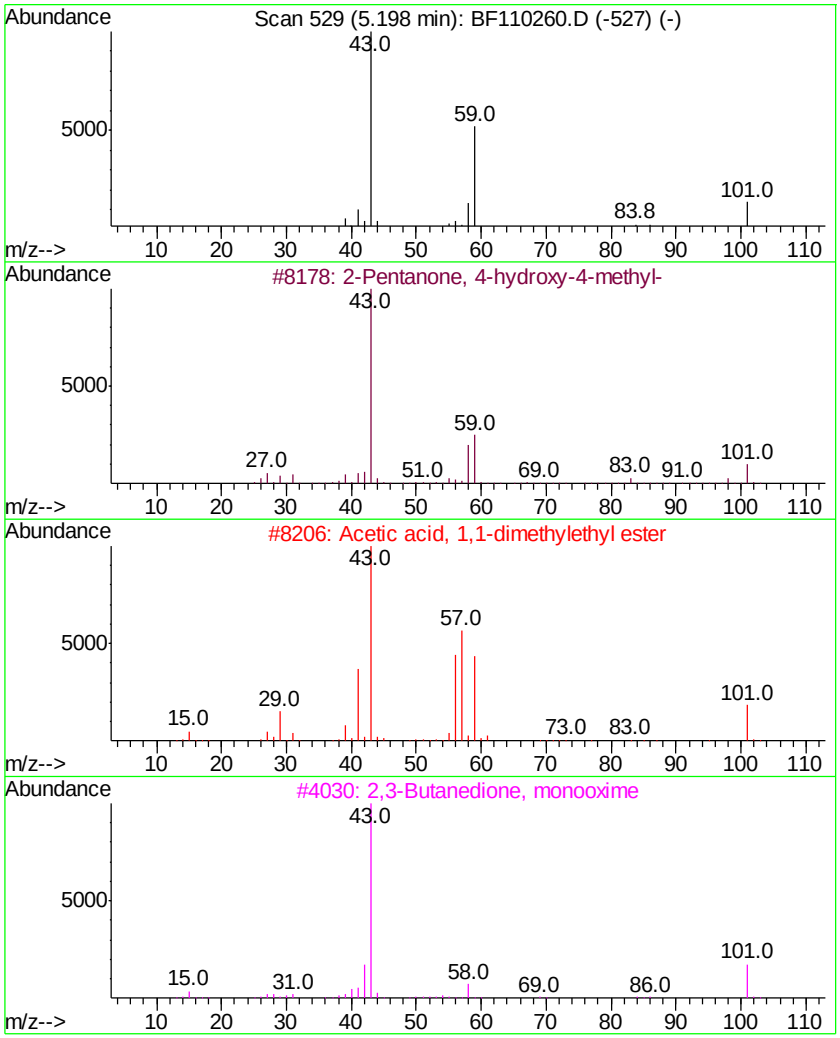
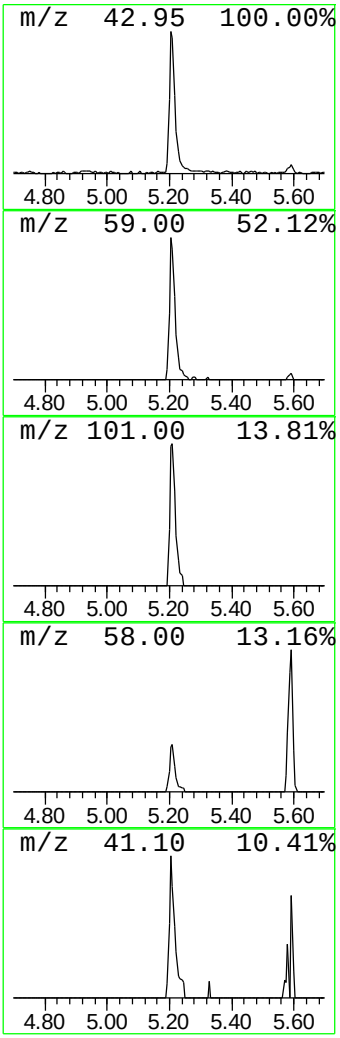
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.79 ng	92101	1,4-Dichlorobenzene-d4	6.97

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	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110260.D
Acq On : 29 Oct 2018 14:12
Operator : JU/SJ
Sample : J5649-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DL-01A

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

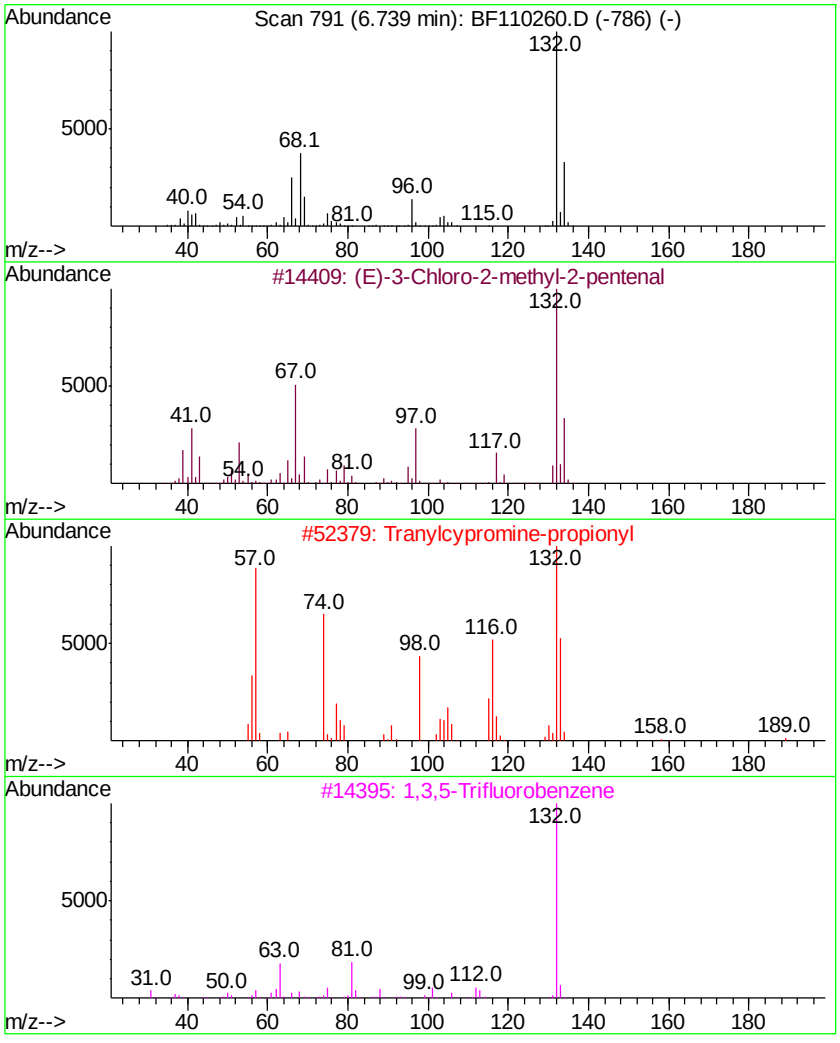
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

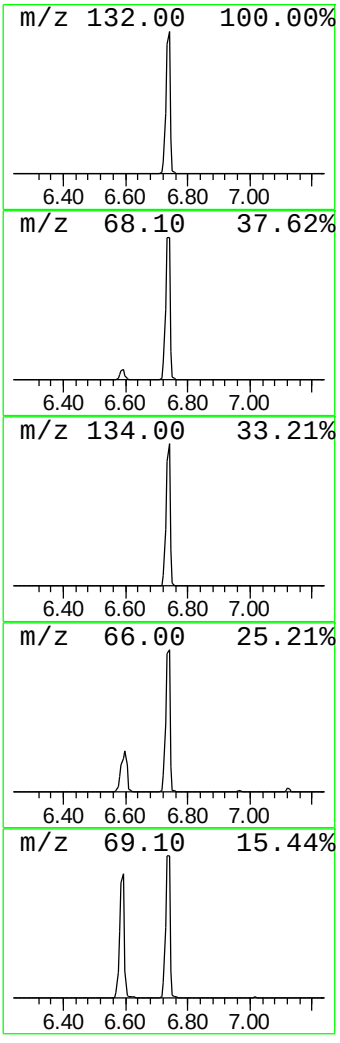
****

Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	67.92 ng	2243710	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110260.D
Acq On : 29 Oct 2018 14:12
Operator : JU/SJ
Sample : J5649-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DL-01A

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

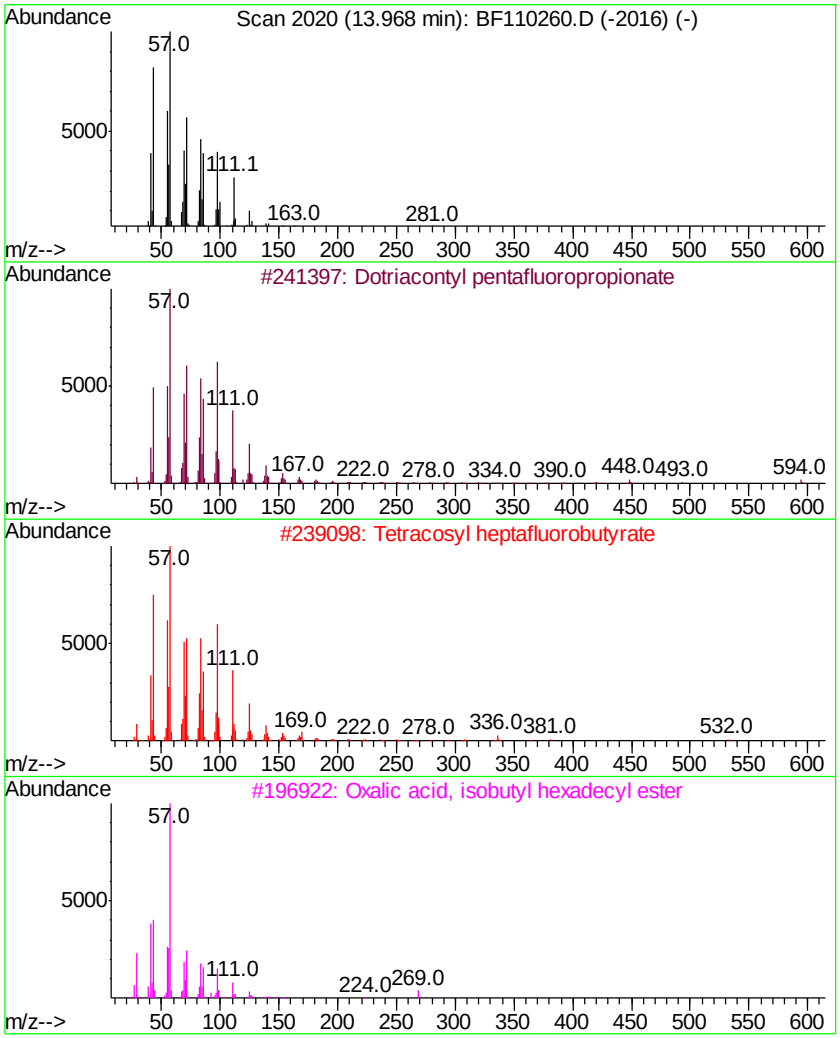
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

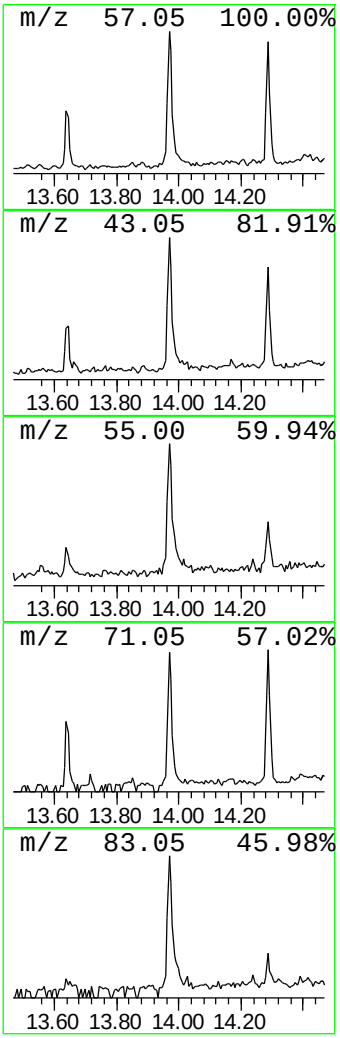
****

Peak Number 5 Dotriacontyl pentafluoropro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	4.16 ng	123719	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	91
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91
5	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110260.D
Acq On : 29 Oct 2018 14:12
Operator : JU/SJ
Sample : J5649-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DL-01A

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

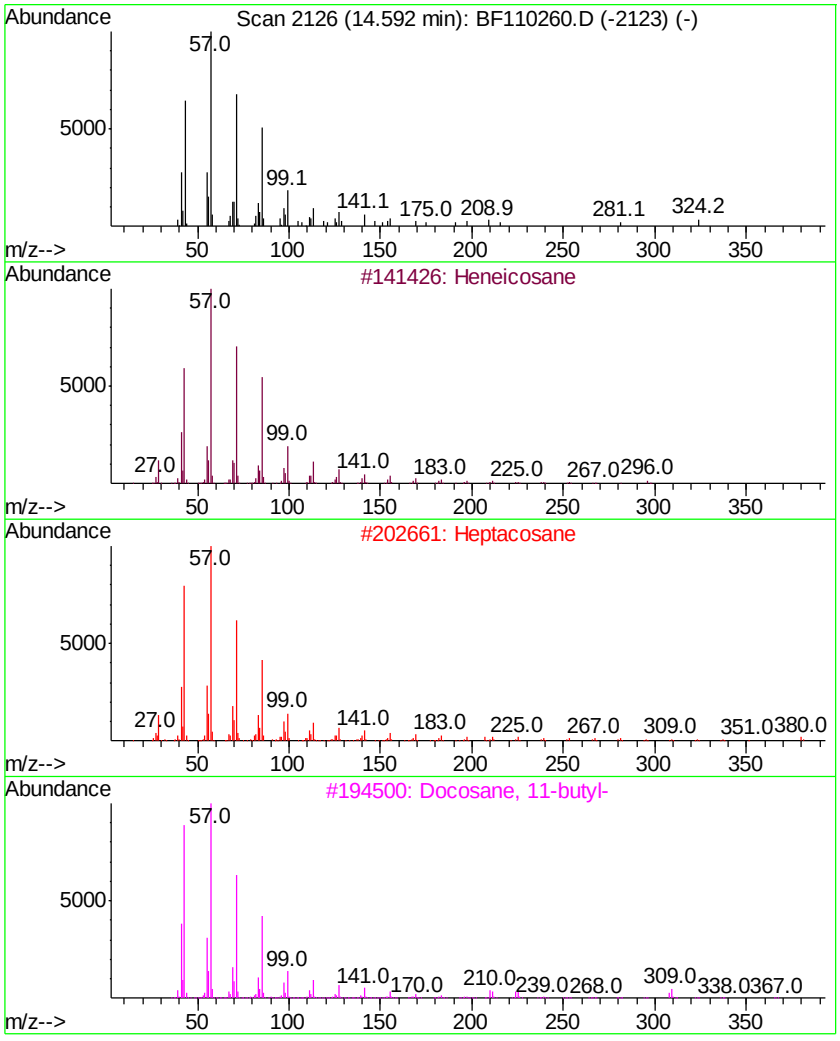
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

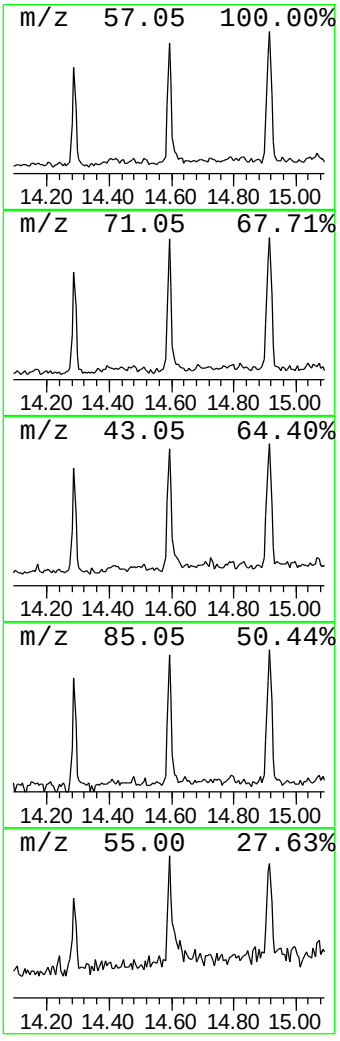
****

Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.96 ng	88022	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

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Sample : J5649-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DL-01A

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

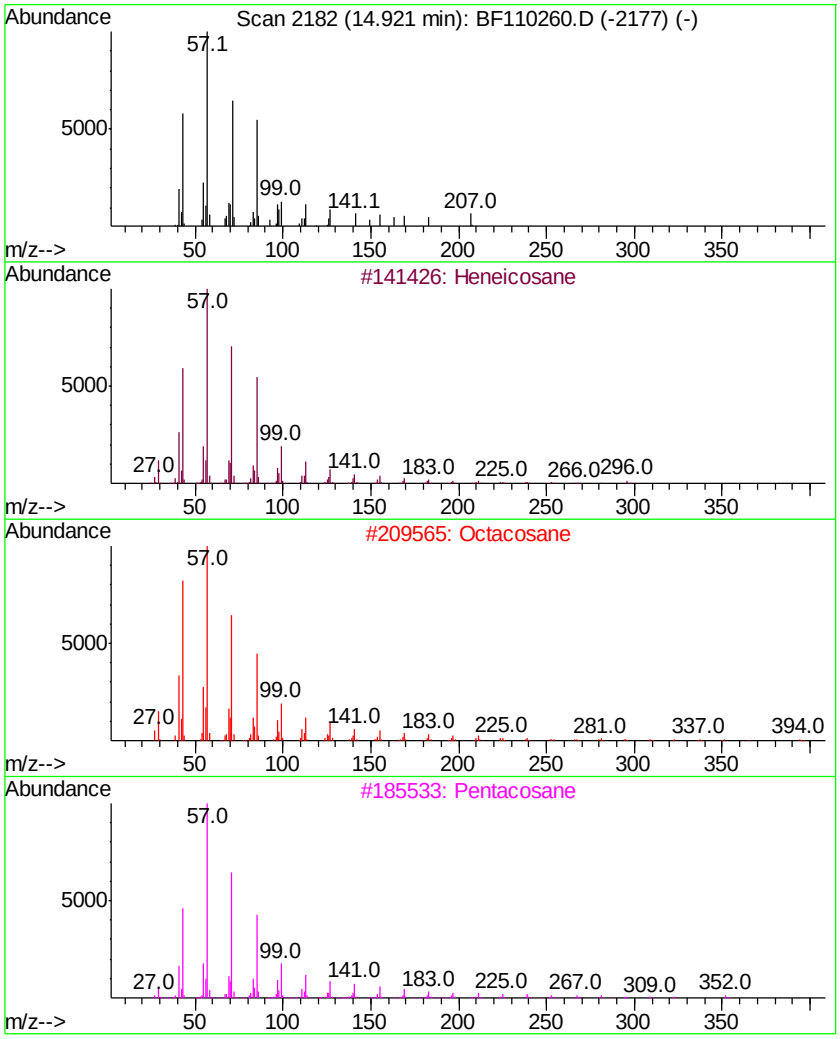
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

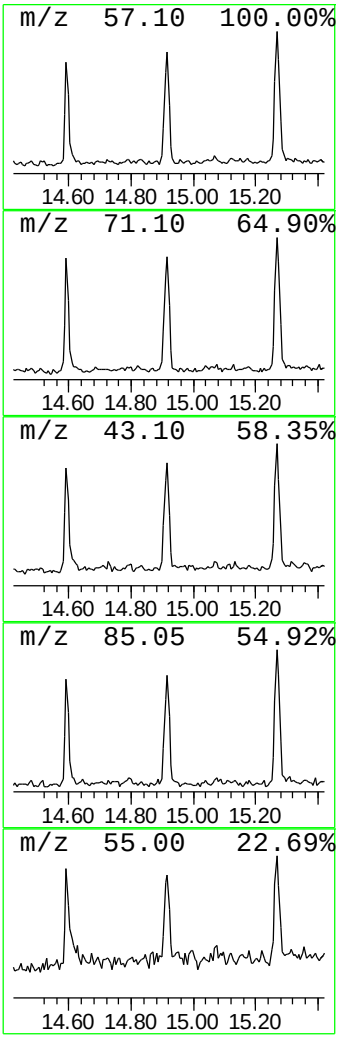
****

Peak Number 7 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.67 ng	79382	Chrysene-d12	14.15

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	Pentacosane	352	C25H52	000629-99-2	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Triacontane	422	C30H62	000638-68-6	91





Library Search Compound Report

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Sample : J5649-01
Misc :
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Instrument : BNA_F
ClientSampleId : DL-01A

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

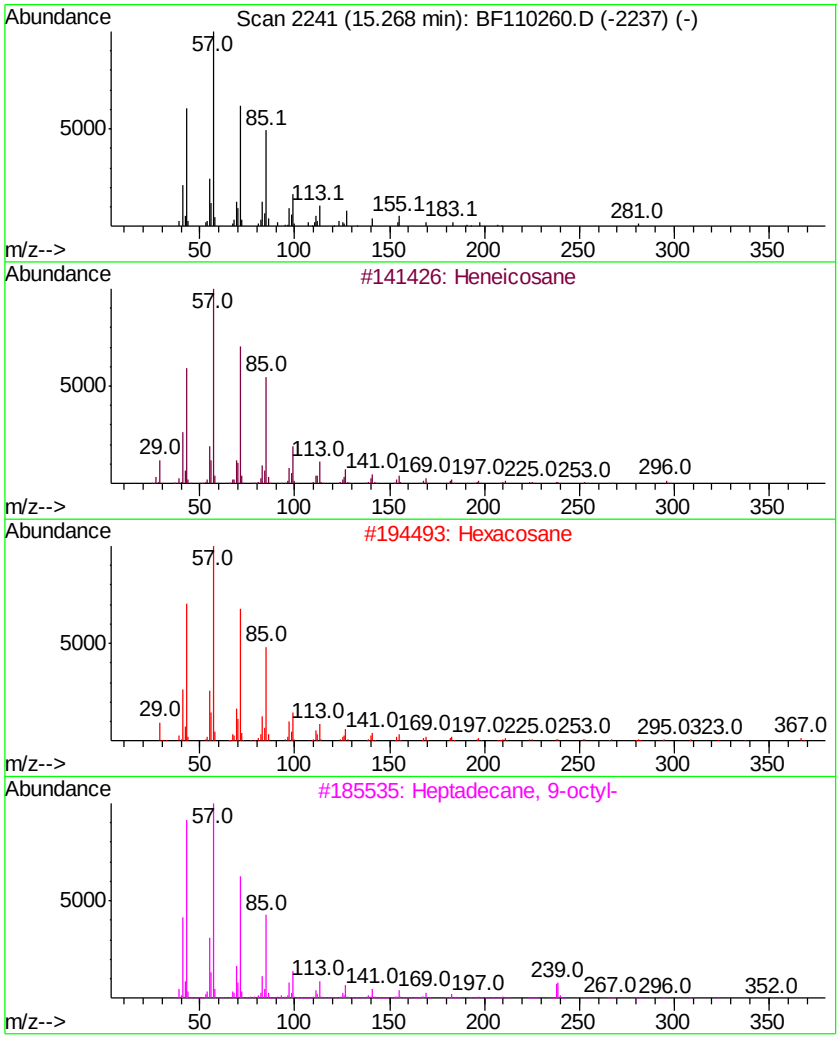
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

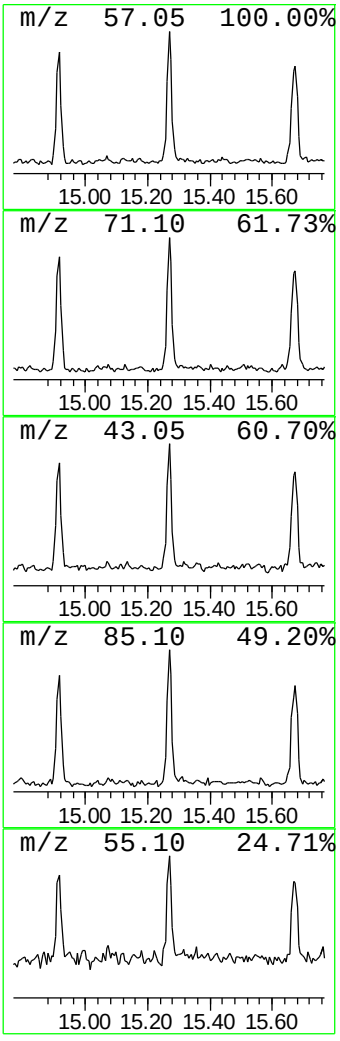
****

Peak Number 8 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	3.13 ng	91717	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Pentacosane	352	C25H52	000629-99-2	91





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ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DL-01A

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

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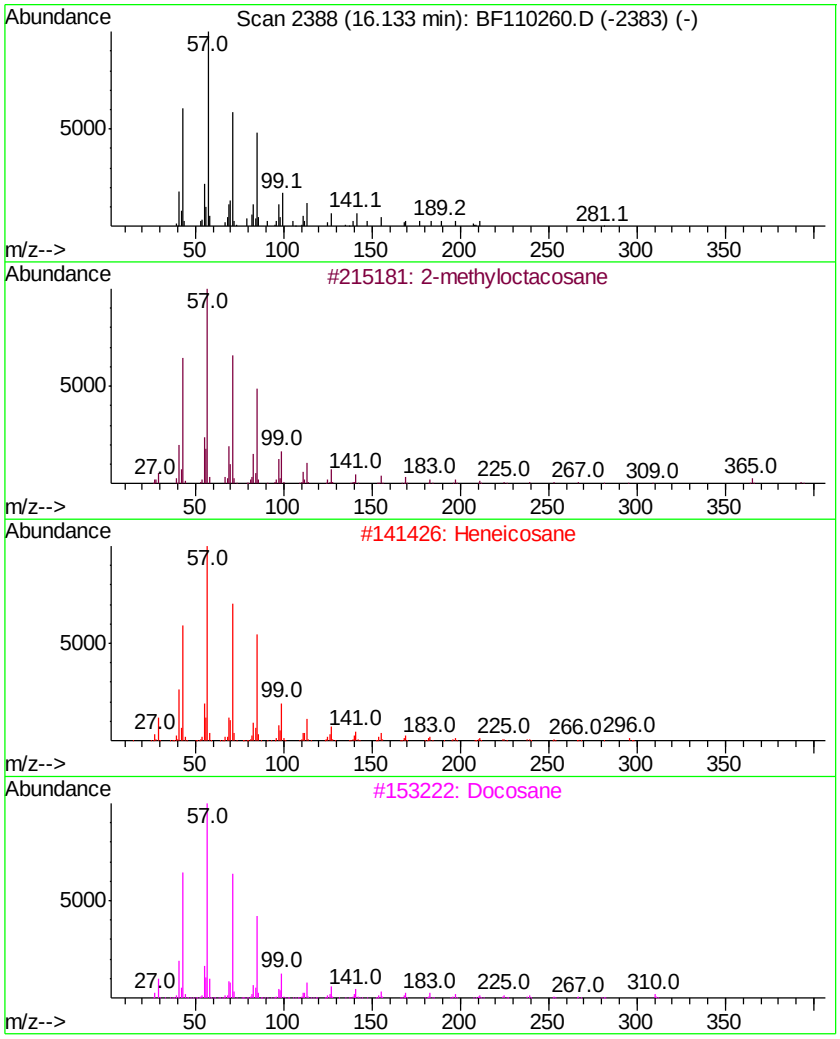
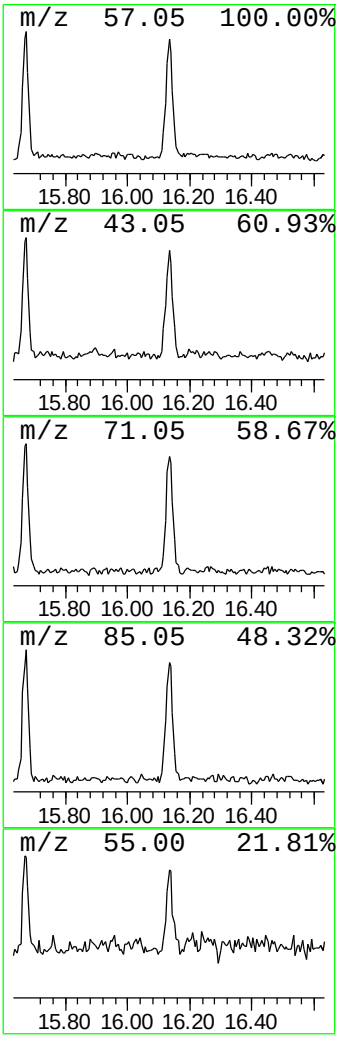
Peak Number 9 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	3.25 ng	95175	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	Docosane	310	C22H46	000629-97-0	86
4	Triacontane	422	C30H62	000638-68-6	86
5	Tetratetracontane	619	C44H90	007098-22-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102918\
Data File : BF110260.D
Acq On : 29 Oct 2018 14:12
Operator : JU/SJ
Sample : J5649-01
Misc :
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Instrument : BNA_F
ClientSampleId : DL-01A

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...	2.31	10.1	ng	332080	1	6.97	660725	20.0
2-Pentanone, 4-hy...	5.20	2.8	ng	92101	1	6.97	660725	20.0
unknown6.74	6.74	67.9	ng	2243710	1	6.97	660725	20.0
Dotriacontyl pent...	13.97	4.2	ng	123719	5	14.15	595503	20.0
Heneicosane	14.59	3.0	ng	88022	5	14.15	595503	20.0
Octacosane	14.92	2.7	ng	79382	5	14.15	595503	20.0
Hexacosane	15.27	3.1	ng	91717	6	15.69	585219	20.0
2-methyloctacosane	16.13	3.3	ng	95175	6	15.69	585219	20.0