LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051319\
Data File : BM020314.D
Acq On : 13 May 2019 13:58
Operator : JU/SJ
Sample : K2763-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P021-SS008-0206-01

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_M\METHODS\8270-BM043019.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	5.346	395	401	416	rBV	869108	1316297	61.04%	8.542%
2	6.928	664	670	683	rBV	812550	1340684	62.17%	8.700%
3	7.293	725	732	741	rBV	894581	1435617	66.57%	9.316%
4	7.757	805	811	817	rBV	175905	285410	13.24%	1.852%
5	8.075	858	865	877	rBV	630586	1013826	47.01%	6.579%
6	8.922	1002	1009	1027	rBV	451382	846518	39.26%	5.493%
7	10.551	1279	1286	1298	rBV	175852	324307	15.04%	2.105%
8	13.022	1699	1706	1716	rBV	918088	1430312	66.33%	9.282%
9	13.863	1843	1849	1860	rBV	153939	221374	10.27%	1.437%
10	14.280	1912	1920	1923	rBV4	10734	24071	1.12%	0.156%
11	14.404	1933	1941	1955	rVB3	288967	449909	20.86%	2.920%
12	15.898	2189	2195	2211	rBV	847998	1312783	60.88%	8.519%
13	17.157	2403	2409	2420	rBV2	363872	545430	25.29%	3.540%
14	18.039	2554	2559	2571	rBV2	90726	150896	7.00%	0.979%
15	19.321	2774	2777	2782	rBV6	21783	32038	1.49%	0.208%
16	19.786	2850	2856	2866	rBV	1738088	2156404	100.00%	13.994%
17	21.045	3066	3070	3077	rBV	161642	200416	9.29%	1.301%
18	21.345	3117	3121	3132	rBV	471655	665765	30.87%	4.320%
19	21.480	3142	3144	3150	rVB5	31371	33091	1.53%	0.215%
20	21.915	3215	3218	3221	rBV2	56765	84146	3.90%	0.546%
21	22.392	3295	3299	3305	rVB2	61510	94107	4.36%	0.611%
22	22.515	3318	3320	3327	rVB	69059	86498	4.01%	0.561%
23	22.627	3336	3339	3344	rVB3	77677	94054	4.36%	0.610%
24	22.903	3382	3386	3390	rBV	138126	177119	8.21%	1.149%
25	22.956	3391	3395	3406	rVB2	123610	221500	10.27%	1.437%
26	23.633	3504	3510	3519	rVB	352348	652084	30.24%	4.232%
27	24.144	3592	3597	3603	rVB	117904	214863	9.96%	1.394%

Sum of corrected areas: 15409519

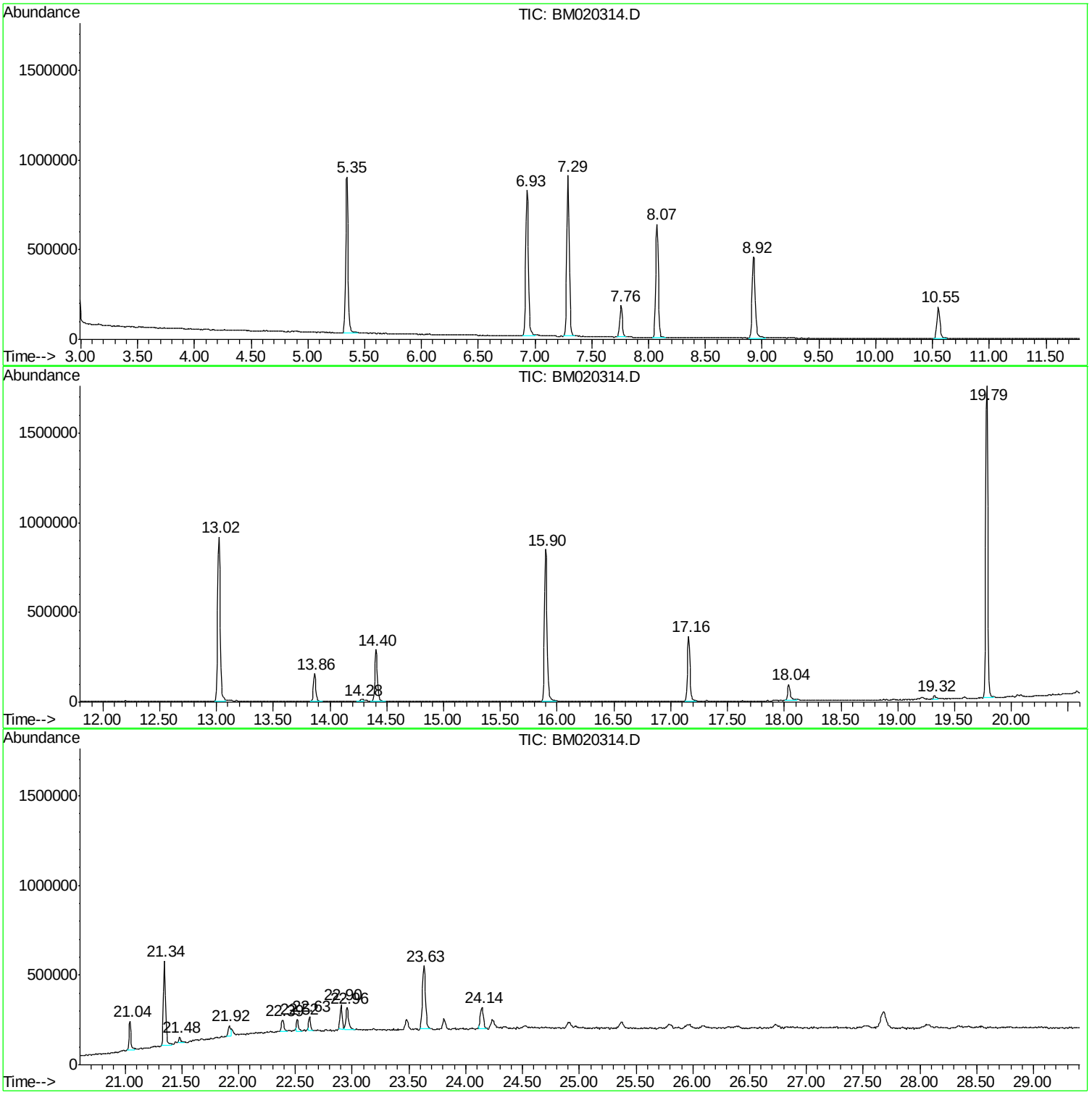
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051319\
Data File : BM020314.D
Acq On : 13 May 2019 13:58
Operator : JU/SJ
Sample : K2763-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P021-SS008-0206-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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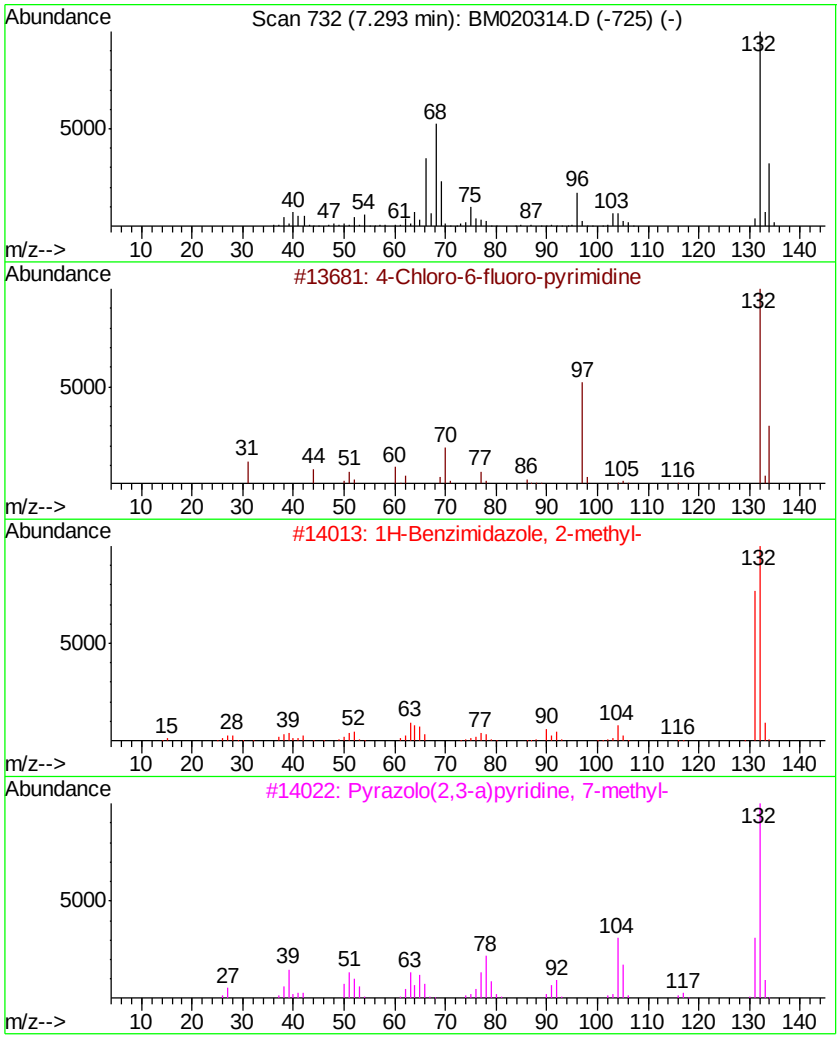
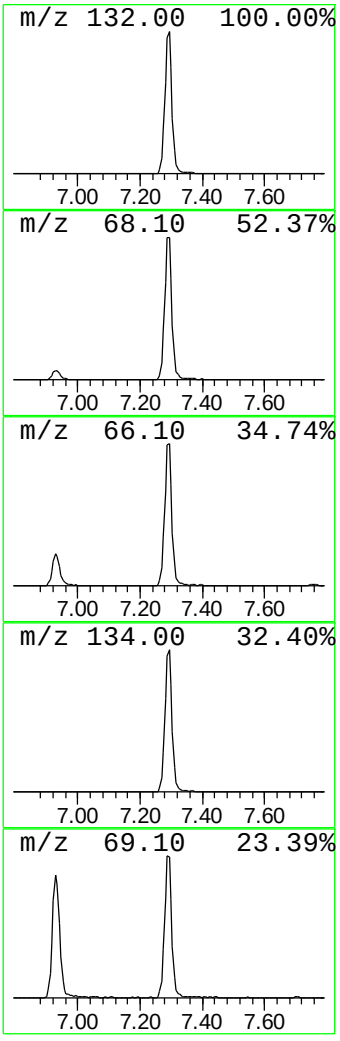
Peak Number 1 unknown7.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	100.60 ng	1435620	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Instrument : BNA_M
ClientSampleId : P021-SS008-0206-01

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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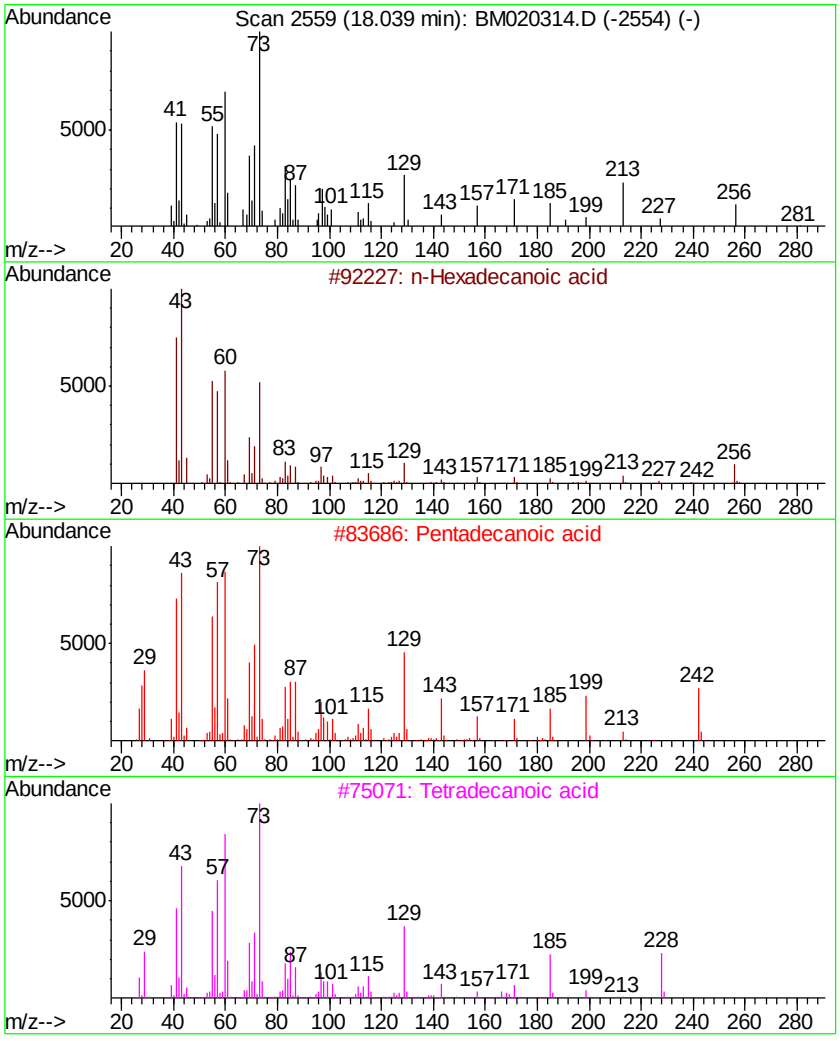
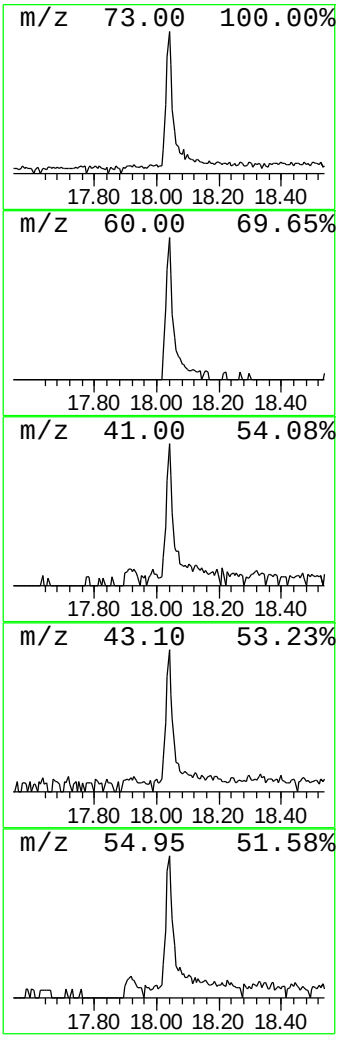
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	5.53 ng	150896	Phenanthrene-d10	17.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4	Undecanoic acid	186	C11H22O2	000112-37-8	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





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Operator : JU/SJ
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Instrument : BNA_M
ClientSampleId : P021-SS008-0206-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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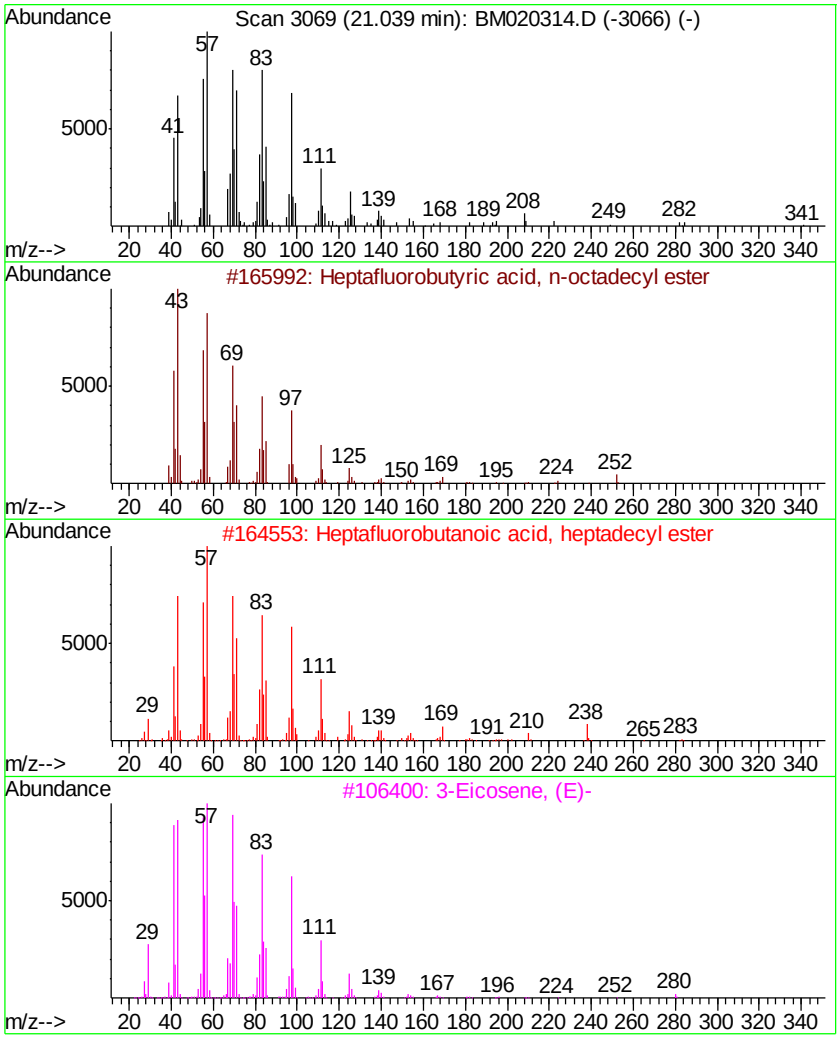
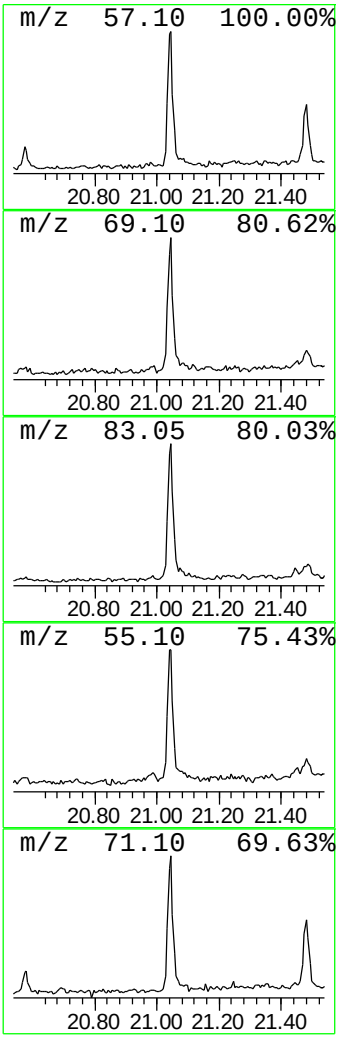
Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	6.02 ng	200416	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	83
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	83





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Instrument : BNA_M
ClientSampleId : P021-SS008-0206-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
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TIC Library : C:\DATABASE\NIST02.L
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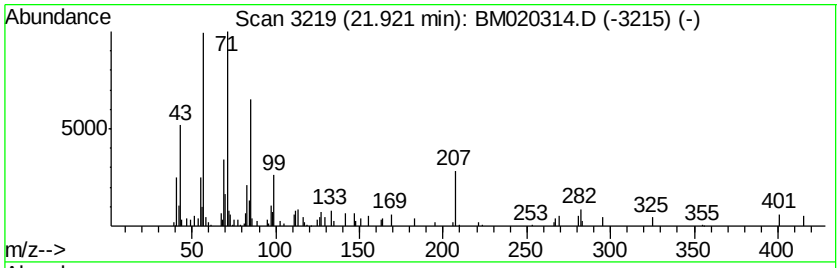
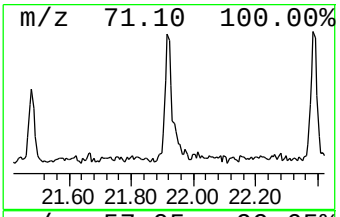
****

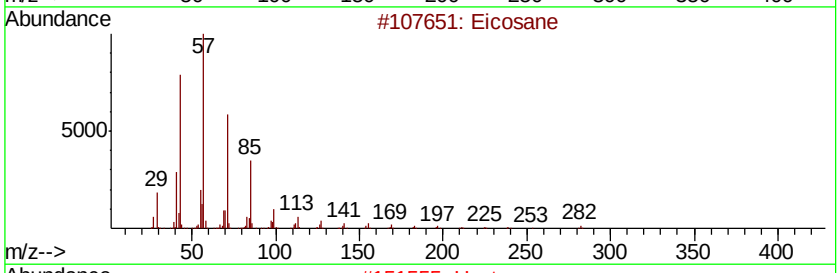
Peak Number 5 Eicosane Concentration Rank 11

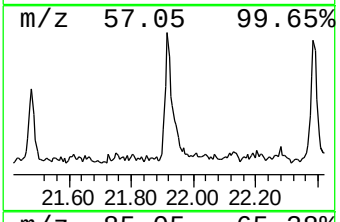
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.92	2.53 ng	84146	Chrysene-d12	21.34

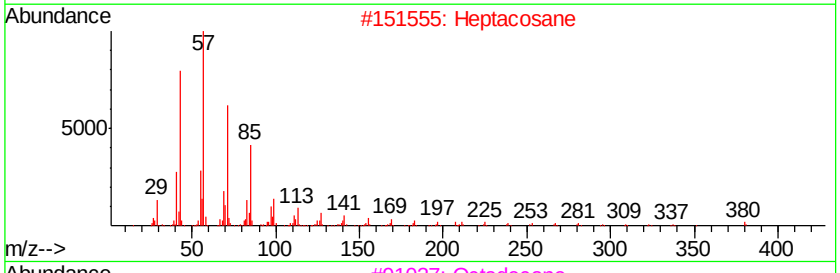
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Heptacosane	380	C27H56	000593-49-7	87
3	Octadecane	254	C18H38	000593-45-3	87
4	10-Methylnonadecane	282	C20H42	056862-62-5	86
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86

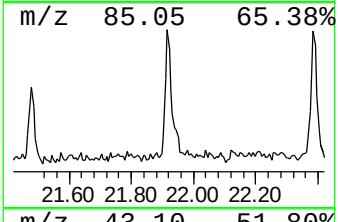


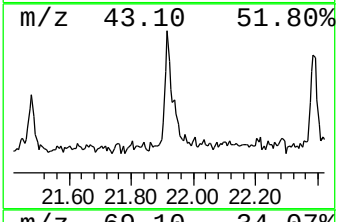


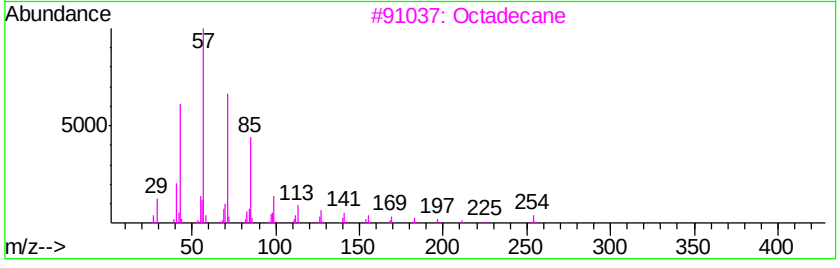


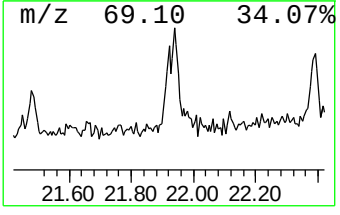












Library Search Compound Report

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Operator : JU/SJ
Sample : K2763-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P021-SS008-0206-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

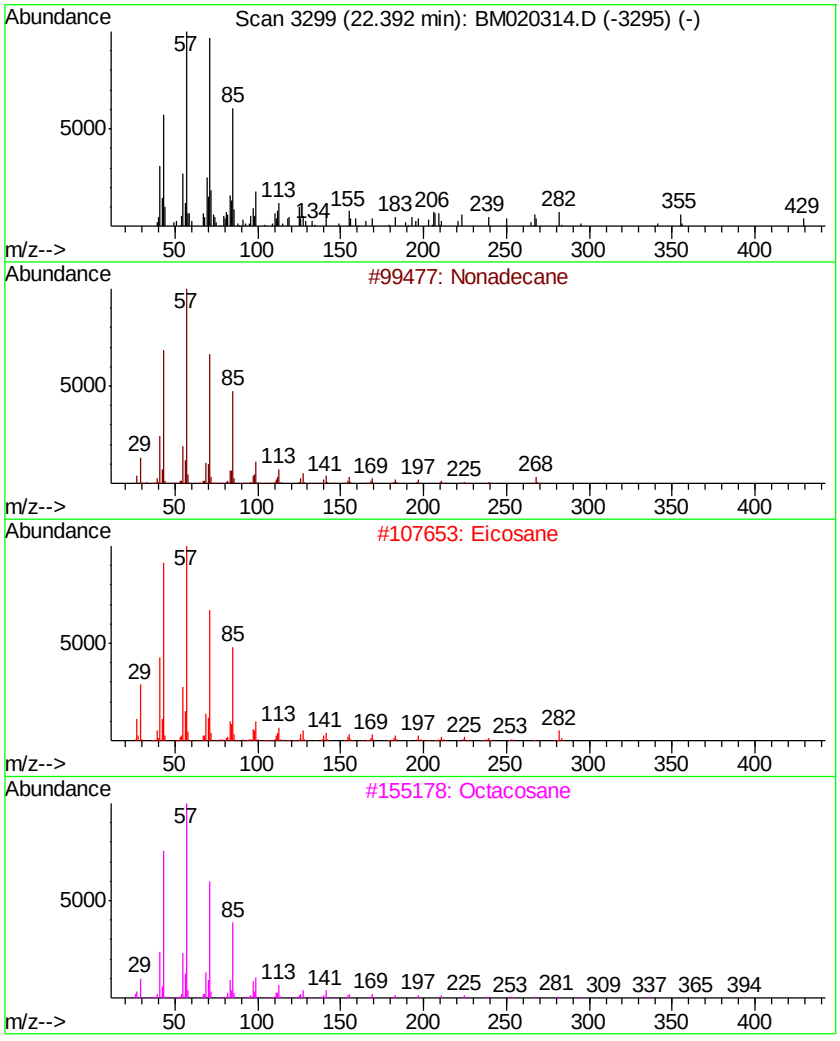
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

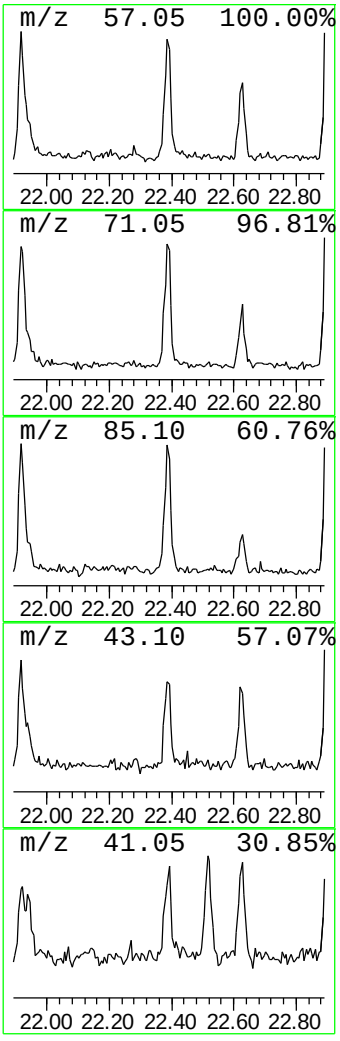
****

Peak Number 6 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.39	2.83 ng	94107	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Eicosane	282	C20H42	000112-95-8	93
3	Octacosane	394	C28H58	000630-02-4	58
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	58
5	Hexadecane	226	C16H34	000544-76-3	58





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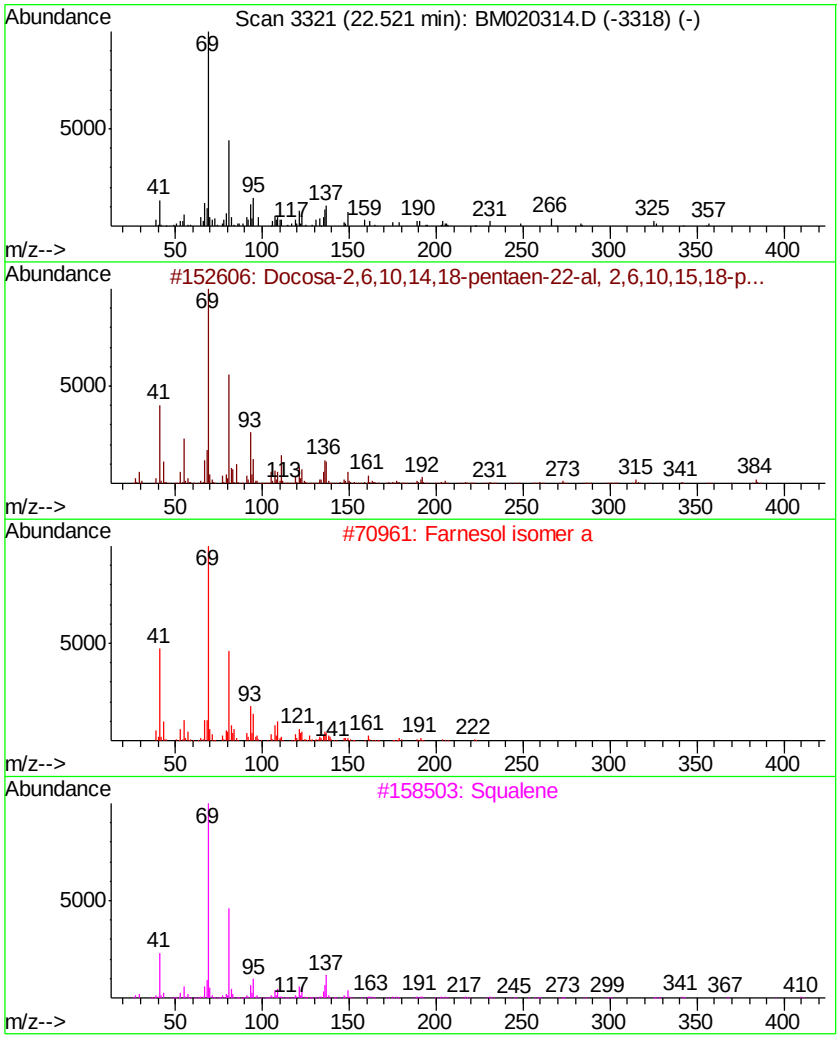
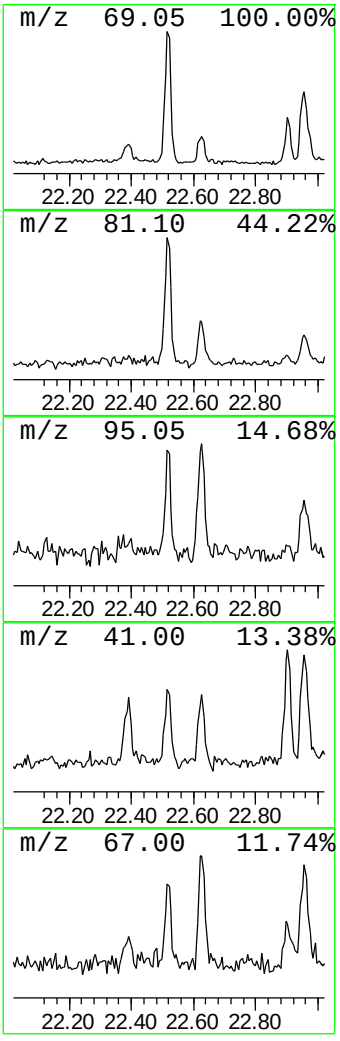
****

Peak Number 7 Docosa-2,6,10,14,18-pentaen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.52	2.65 ng	86498	Perylene-d12	23.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	58
2	Farnesol isomer a	222	C15H26O	1000108-92-4	58
3	Squalene	410	C30H50	007683-64-9	53
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	50
5	1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	50





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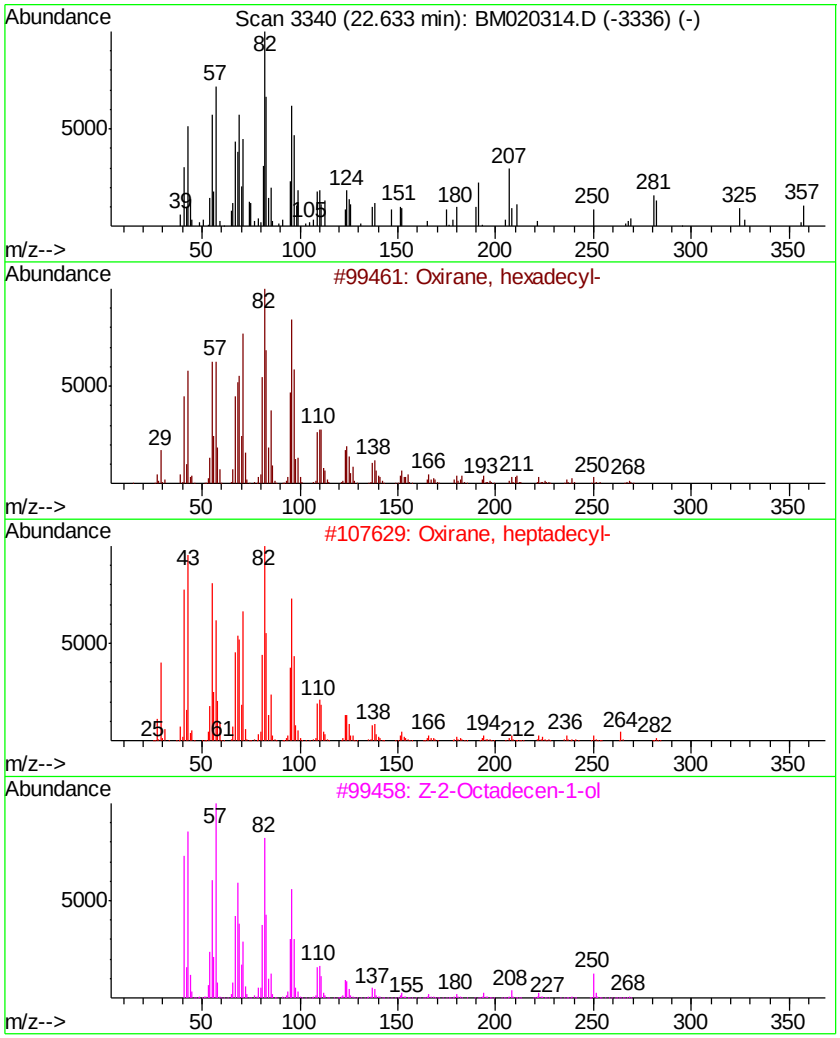
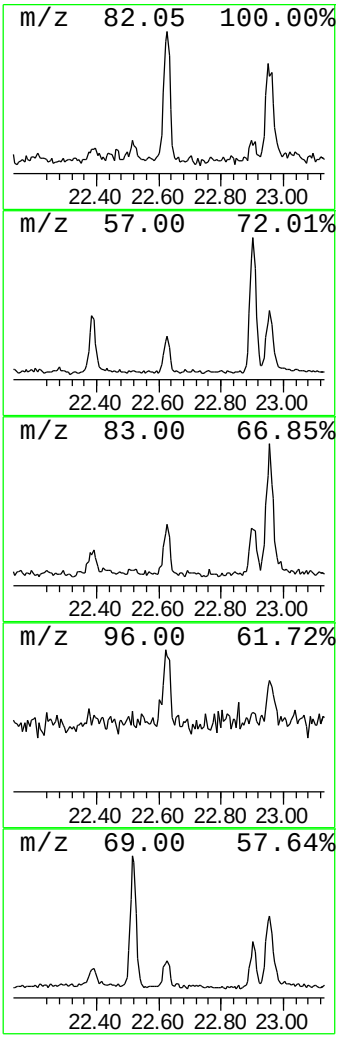
****

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.63	2.88 ng	94054	Perylene-d12	23.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	52
3	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	49
4	1,13-Tridecanediol, diacetate	300	C17H32O4	042236-70-4	46
5	E-3-Pentadecen-2-ol	226	C15H30O	1000130-83-8	46





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Instrument : BNA_M
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TIC Library : C:\DATABASE\NIST02.L
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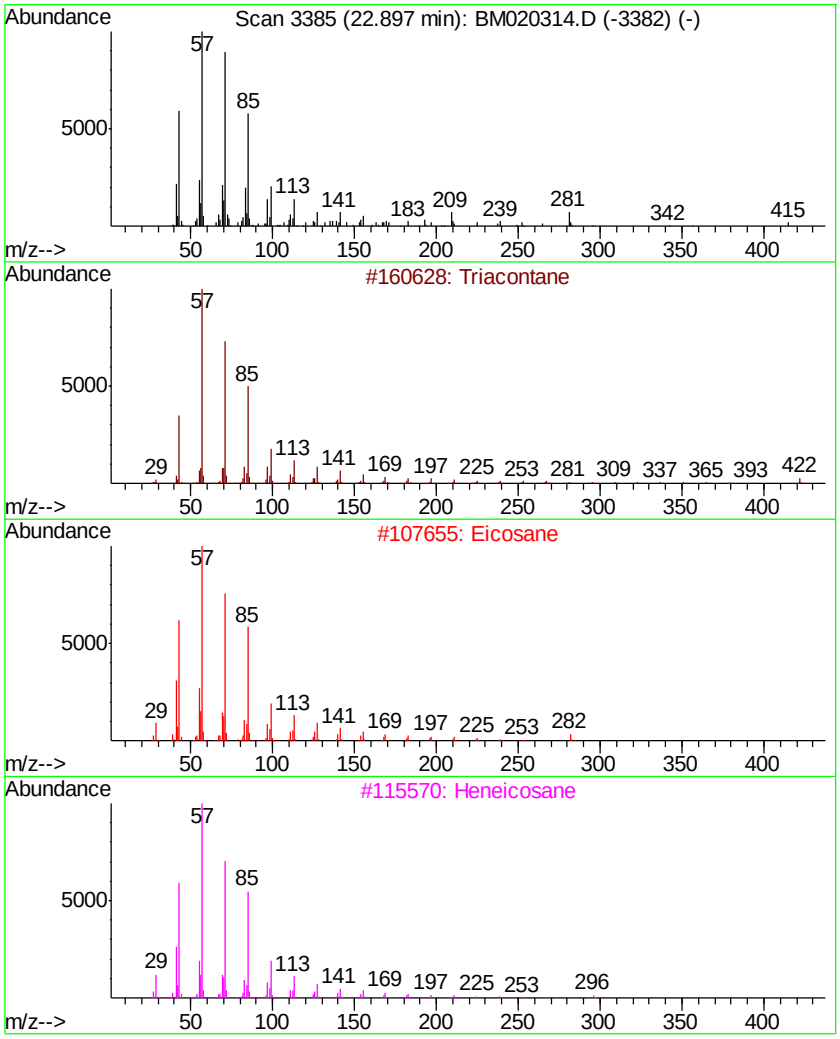
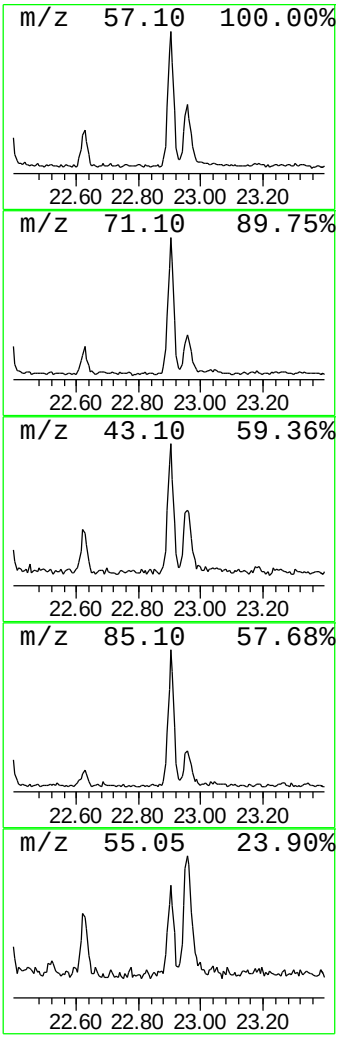
Peak Number 9 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.90	5.43 ng	177119	Perylene-d12	23.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	90
2	Eicosane	282	C20H42	000112-95-8	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	83
5	Octacosane	394	C28H58	000630-02-4	81





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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P021-SS008-0206-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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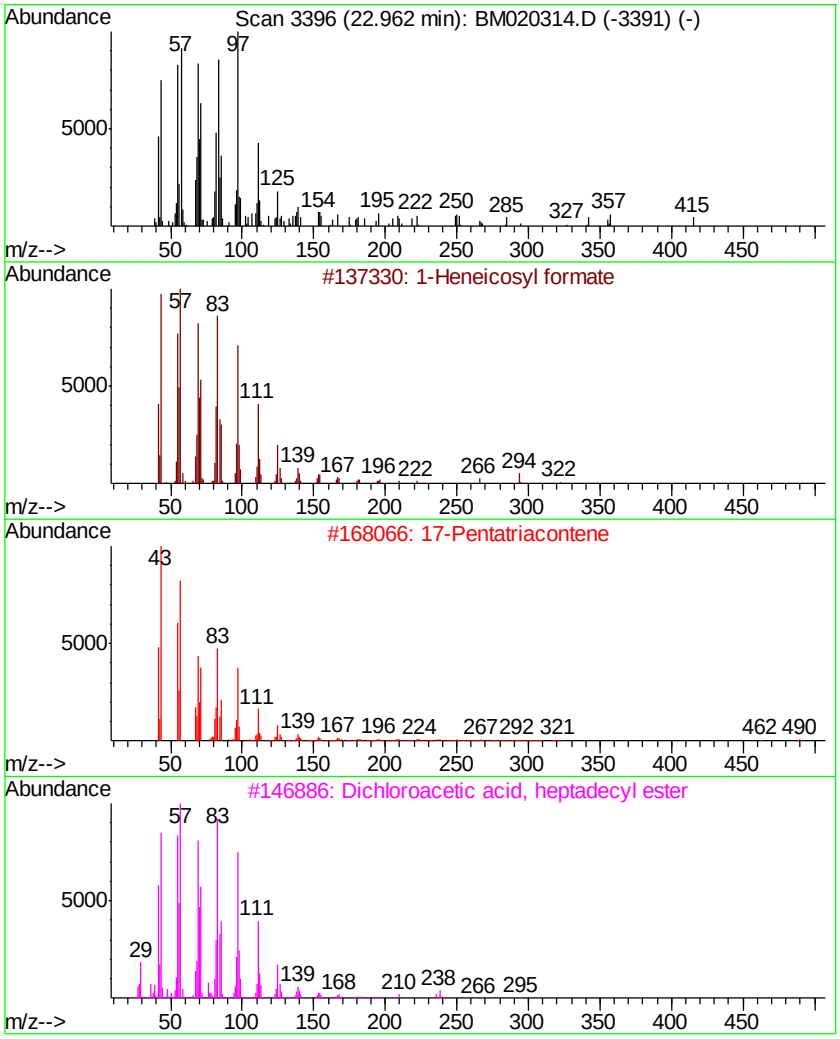
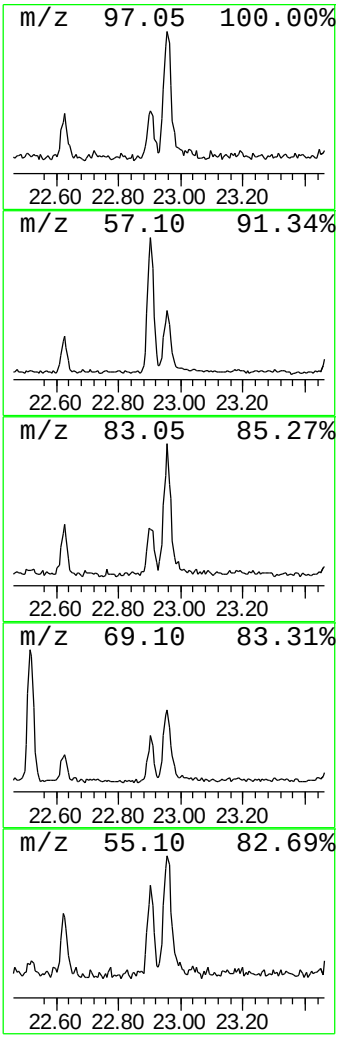
Peak Number 10 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.96	6.79 ng	221500	Perylene-d12	23.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
2	17-Pentatriacontene	491	C35H70	006971-40-0	87
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	86
4	1-Octadecene	252	C18H36	000112-88-9	83
5	1-Pentadecene	210	C15H30	013360-61-7	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051319\
Data File : BM020314.D
Acq On : 13 May 2019 13:58
Operator : JU/SJ
Sample : K2763-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P021-SS008-0206-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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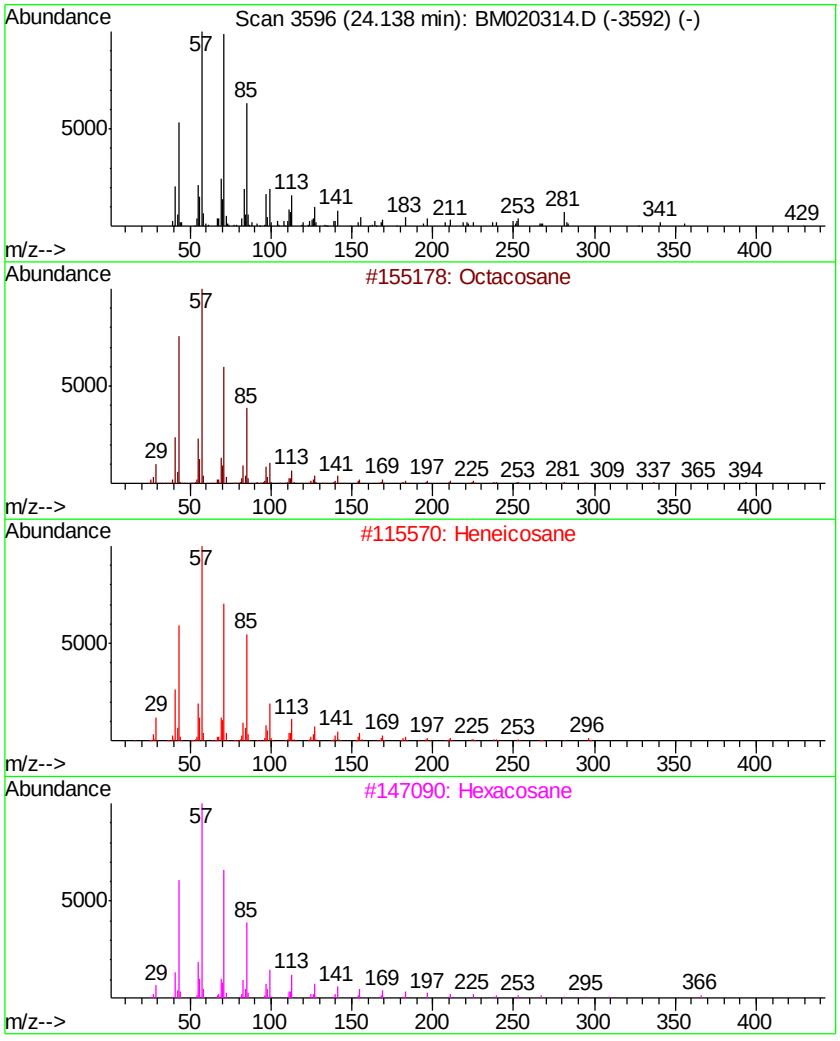
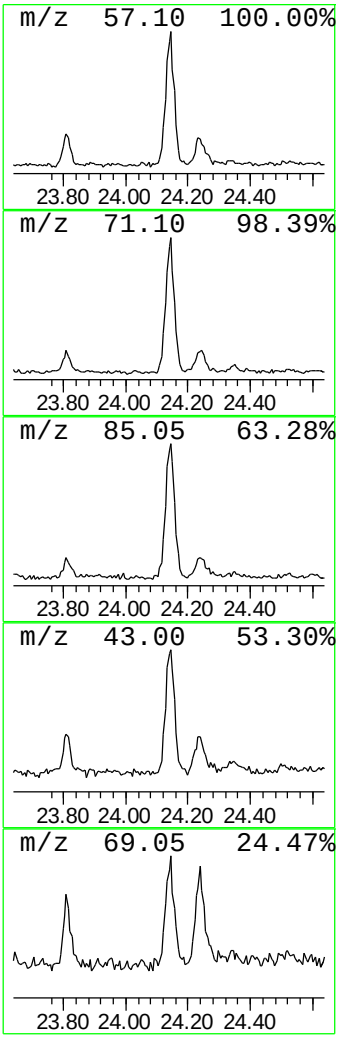
Peak Number 11 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.14	6.59 ng	214863	Perylene-d12	23.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexacosane	366	C26H54	000630-01-3	86
4	Hentriacontane	437	C31H64	000630-04-6	83
5	Nonacosane	408	C29H60	000630-03-5	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM051319\
Data File : BM020314.D
Acq On : 13 May 2019 13:58
Operator : JU/SJ
Sample : K2763-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P021-SS008-0206-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.29	7.29	100.6	ng	1435620	1	7.76	285410	20.0
n-Hexadecanoic acid	18.04	5.5	ng	150896	4	17.16	545430	20.0
Heptafluorobutyri...	21.04	6.0	ng	200416	5	21.34	665765	20.0
Eicosane	21.92	2.5	ng	84146	5	21.34	665765	20.0
Nonadecane	22.39	2.8	ng	94107	5	21.34	665765	20.0
Docosa-2,6,10,14,...	22.52	2.6	ng	86498	6	23.63	652084	20.0
Oxirane, hexadecyl-	22.63	2.9	ng	94054	6	23.63	652084	20.0
Triacontane	22.90	5.4	ng	177119	6	23.63	652084	20.0
1-Heneicosyl formate	22.96	6.8	ng	221500	6	23.63	652084	20.0
Octacosane	24.14	6.6	ng	214863	6	23.63	652084	20.0