LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051219\
Data File : BM020293.D
Acq On : 12 May 2019 11:56
Operator : JU/SJ
Sample : K2768-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P026-SS014-0612-01

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	5.345	395	401	414	rBV	1180003	1724876	60.28%	8.974%
2	6.934	663	671	685	rBV	1065267	1774261	62.00%	9.231%
3	7.292	726	732	746	rBV	1142697	1848830	64.61%	9.619%
4	7.763	806	812	820	rBV	206371	331063	11.57%	1.722%
5	8.081	859	866	882	rVB	857736	1393601	48.70%	7.251%
6	8.933	1003	1011	1030	rBV	603568	1086743	37.98%	5.654%
7	10.557	1280	1287	1303	rBV	213273	385735	13.48%	2.007%
8	13.027	1700	1707	1721	rBV	1255074	1926543	67.33%	10.023%
9	13.868	1843	1850	1863	rBV	137129	197742	6.91%	1.029%
10	14.410	1935	1942	1952	rBV2	331698	514183	17.97%	2.675%
11	15.904	2190	2196	2213	rBV	1237625	1778253	62.14%	9.252%
12	17.156	2403	2409	2421	rBV2	413891	659506	23.05%	3.431%
13	18.039	2551	2559	2569	rBV	84041	132239	4.62%	0.688%
14	19.321	2774	2777	2782	rBV2	25585	35145	1.23%	0.183%
15	19.786	2851	2856	2865	rBV	2326730	2861555	100.00%	14.888%
16	21.044	3066	3070	3074	rBV	137069	182807	6.39%	0.951%
17	21.350	3116	3122	3133	rBV	641899	917029	32.05%	4.771%
18	21.921	3216	3219	3220	rBV	59718	60418	2.11%	0.314%
19	21.944	3220	3223	3228	rVB	106046	147304	5.15%	0.766%
20	22.515	3317	3320	3327	rVB	114596	158749	5.55%	0.826%
21	22.903	3382	3386	3391	rBV	82354	122829	4.29%	0.639%
22	23.632	3503	3510	3519	rVB	507792	981066	34.28%	5.104%

Sum of corrected areas: 19220477

LSC Report - Integrated Chromatogram

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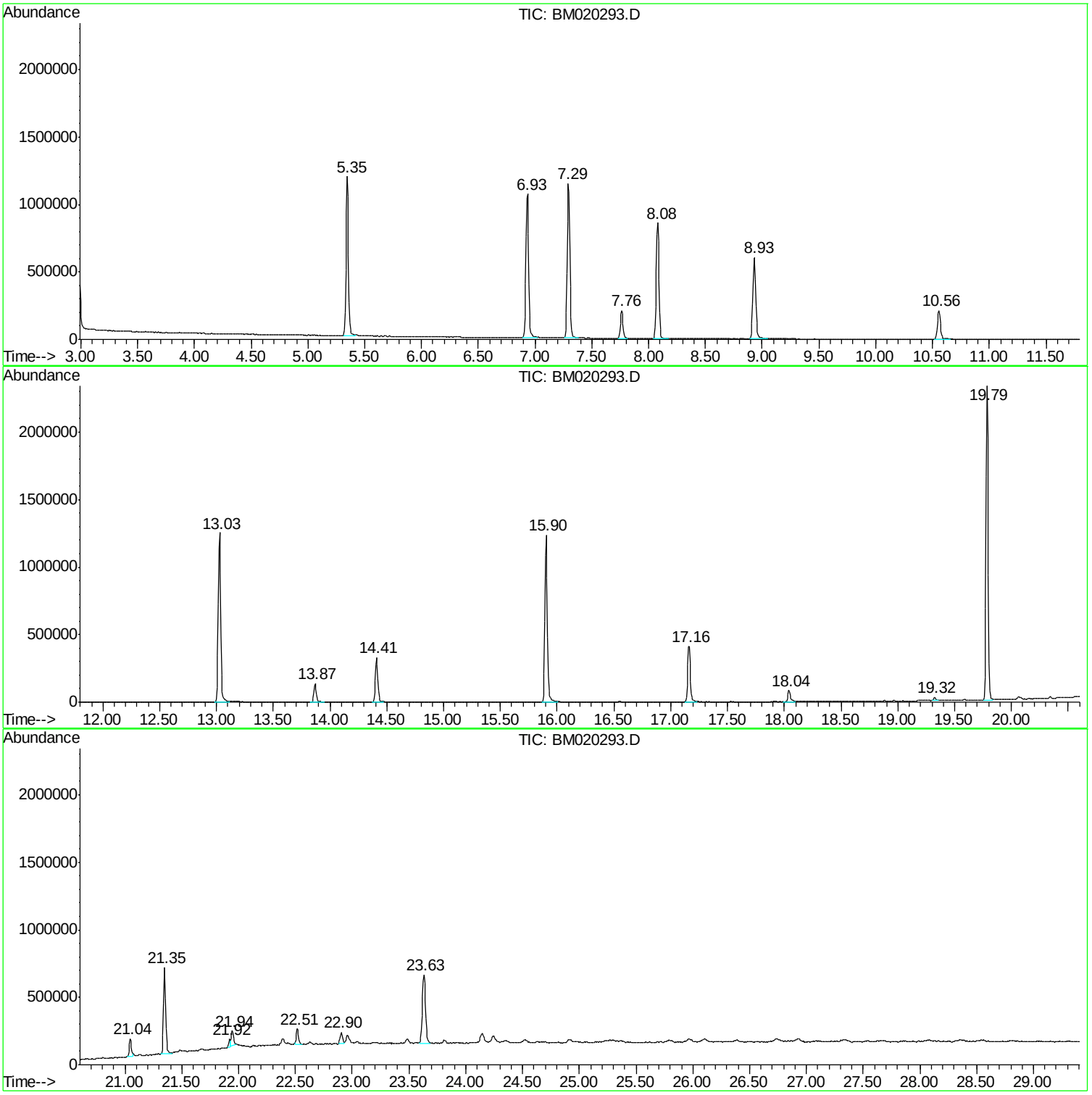
Instrument : BNA_M
ClientSampleId : P026-SS014-0612-01

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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Operator : JU/SJ
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Instrument : BNA_M
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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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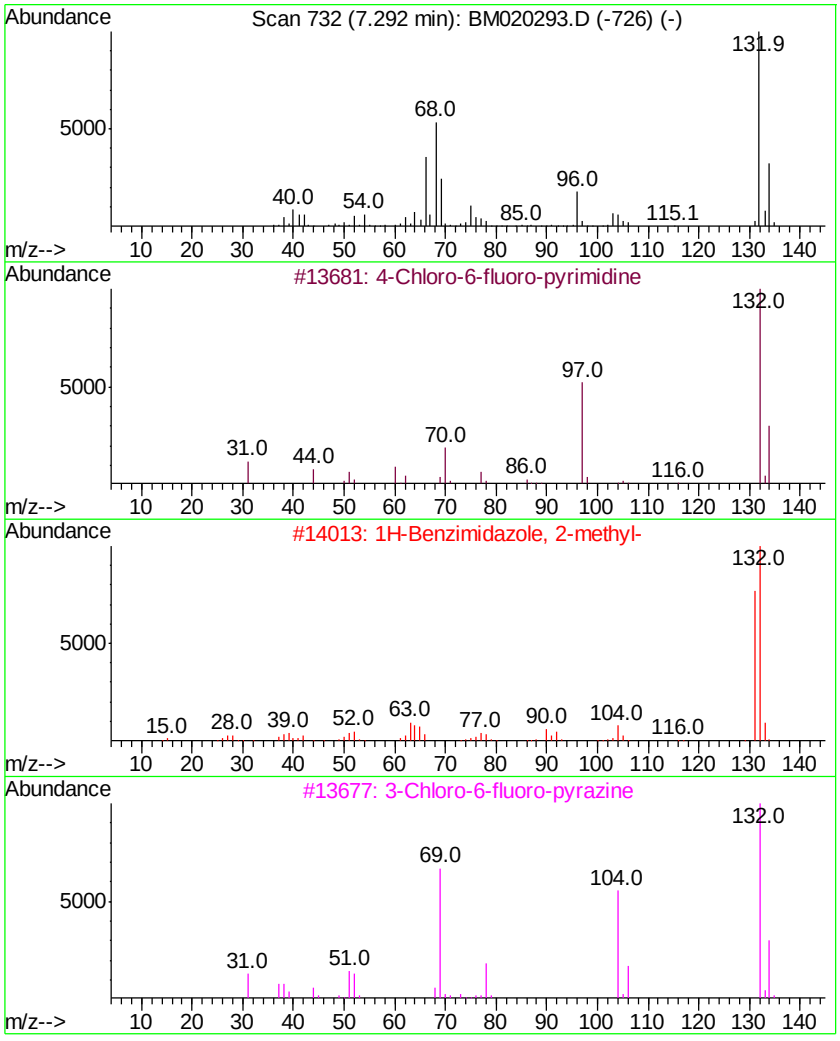
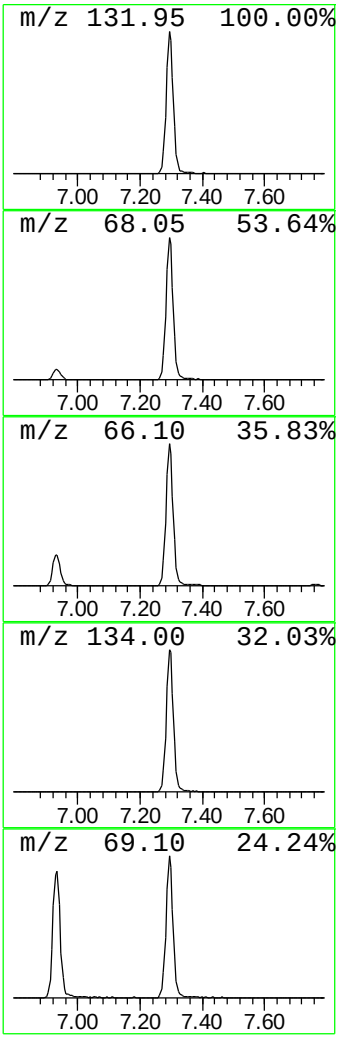
Peak Number 1 unknown7.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	111.69 ng	1848830	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	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12





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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P026-SS014-0612-01

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

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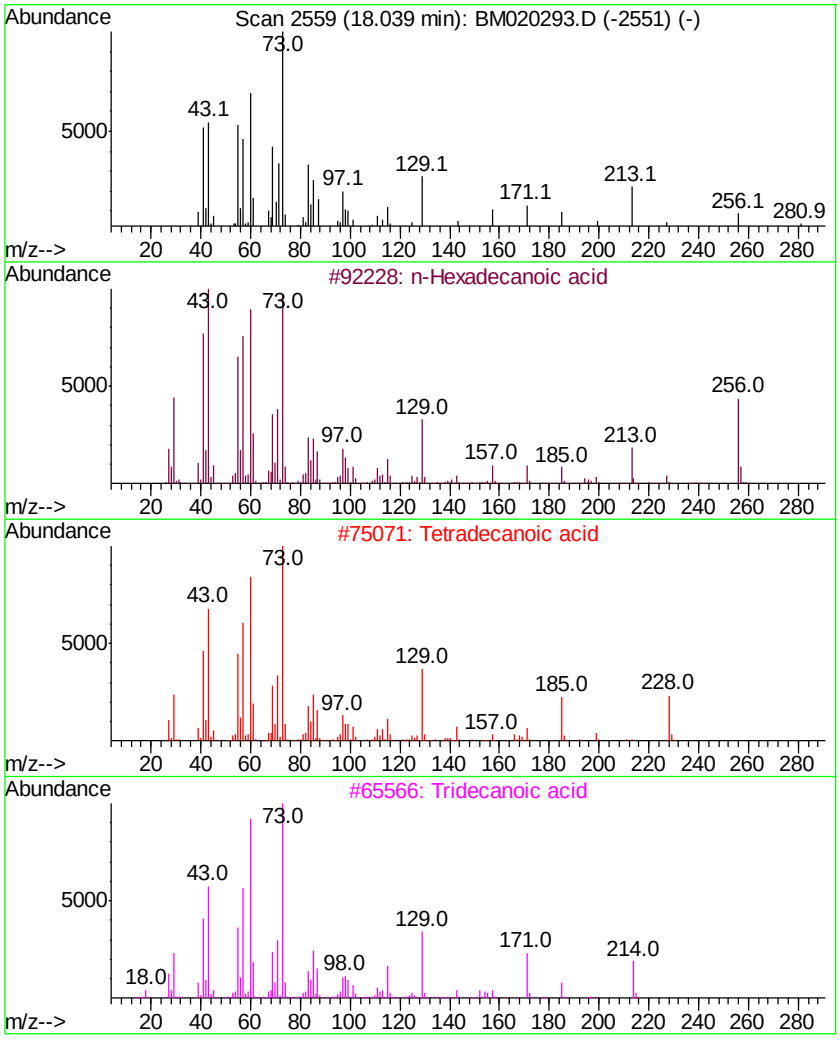
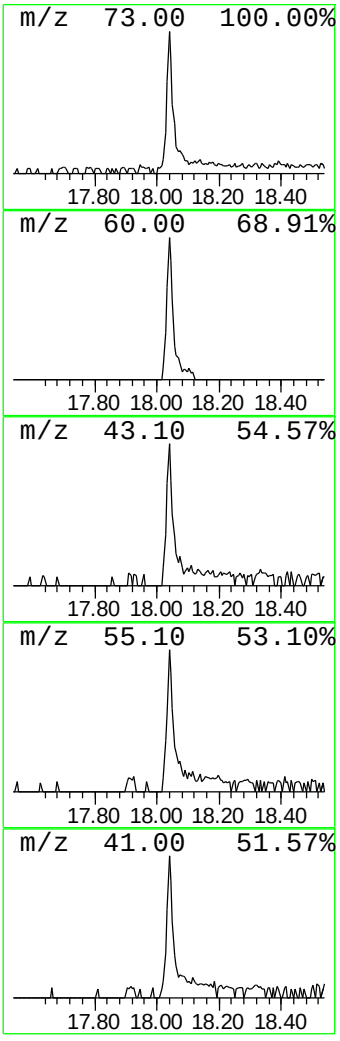
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	4.01 ng	132239	Phenanthrene-d10	17.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3	Tridecanoic acid	214	C13H26O2	000638-53-9	50
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	40





Library Search Compound Report

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Acq On : 12 May 2019 11:56
Operator : JU/SJ
Sample : K2768-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P026-SS014-0612-01

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

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TIC Integration Parameters: LSCINT.P

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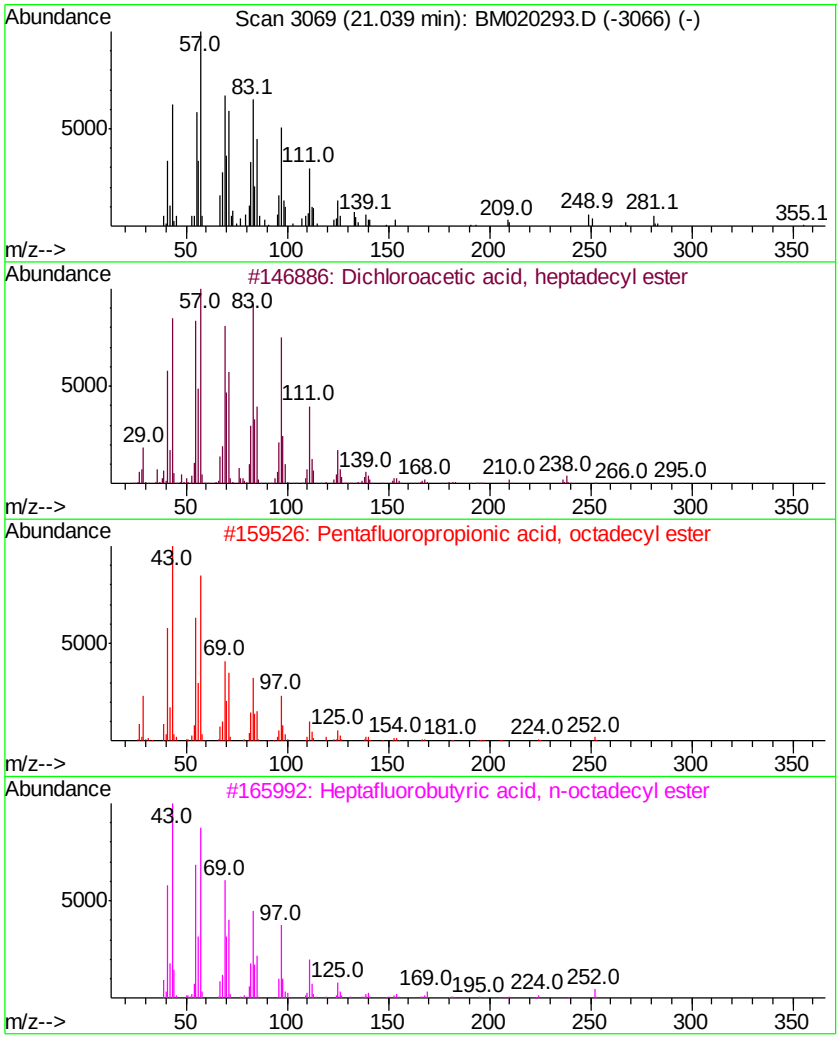
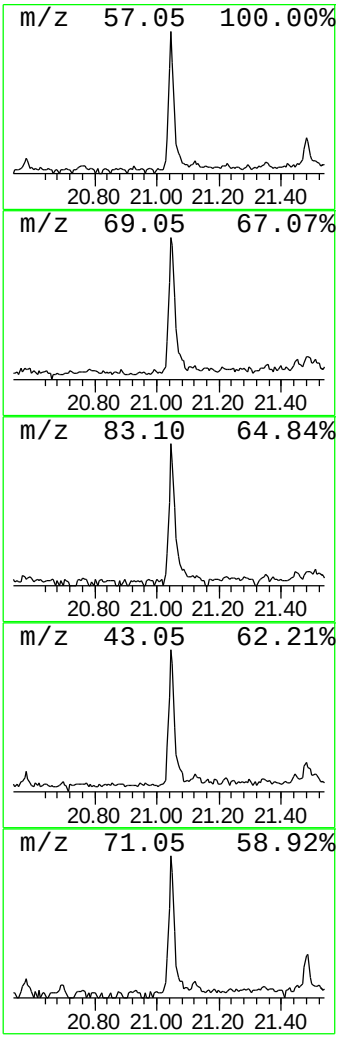
Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	3.99 ng	182807	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	90
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	86





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Operator : JU/SJ
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P026-SS014-0612-01

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
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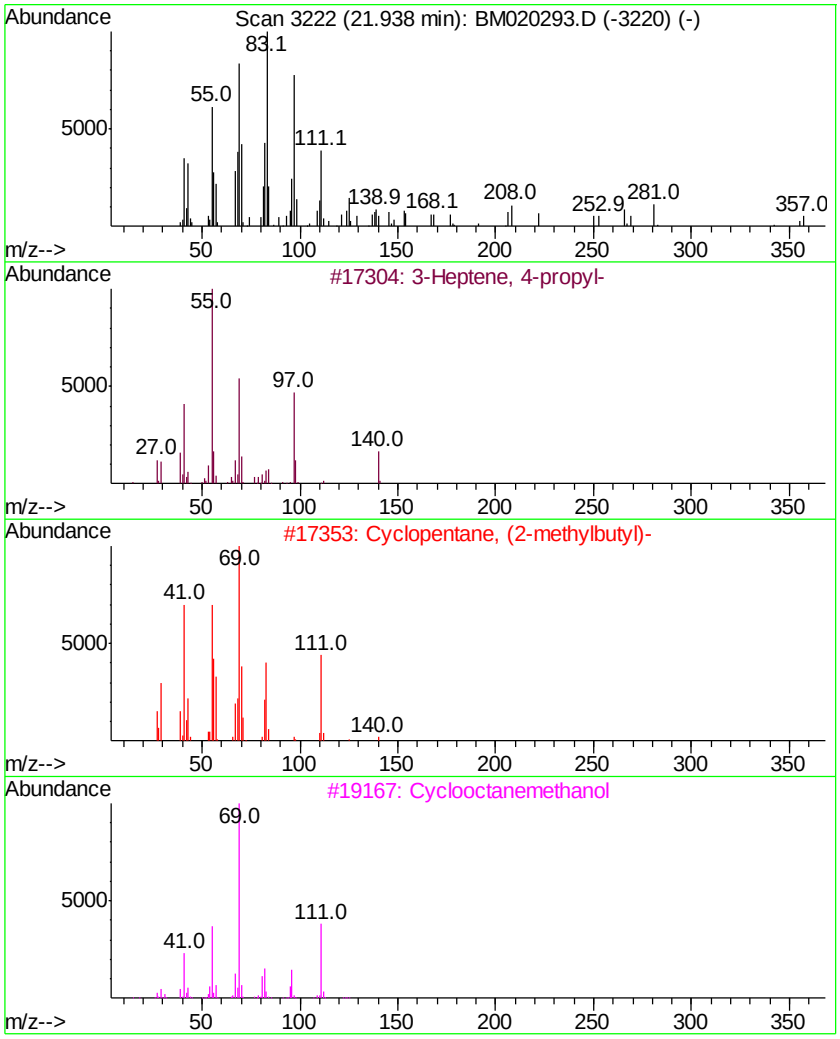
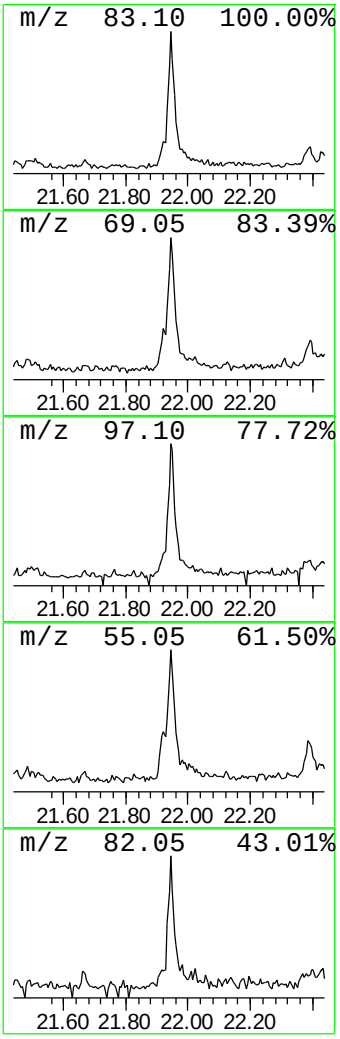
Peak Number 5 unknown21.94 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.94	3.21 ng	147304	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptene, 4-propyl-	140	C10H20	004485-13-6	38
2	Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	27
3	Cyclooctanemethanol	142	C9H18O	003637-63-6	27
4	Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	25
5	Cyclohexane, propyl-	126	C9H18	001678-92-8	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051219\
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Sample : K2768-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P026-SS014-0612-01

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

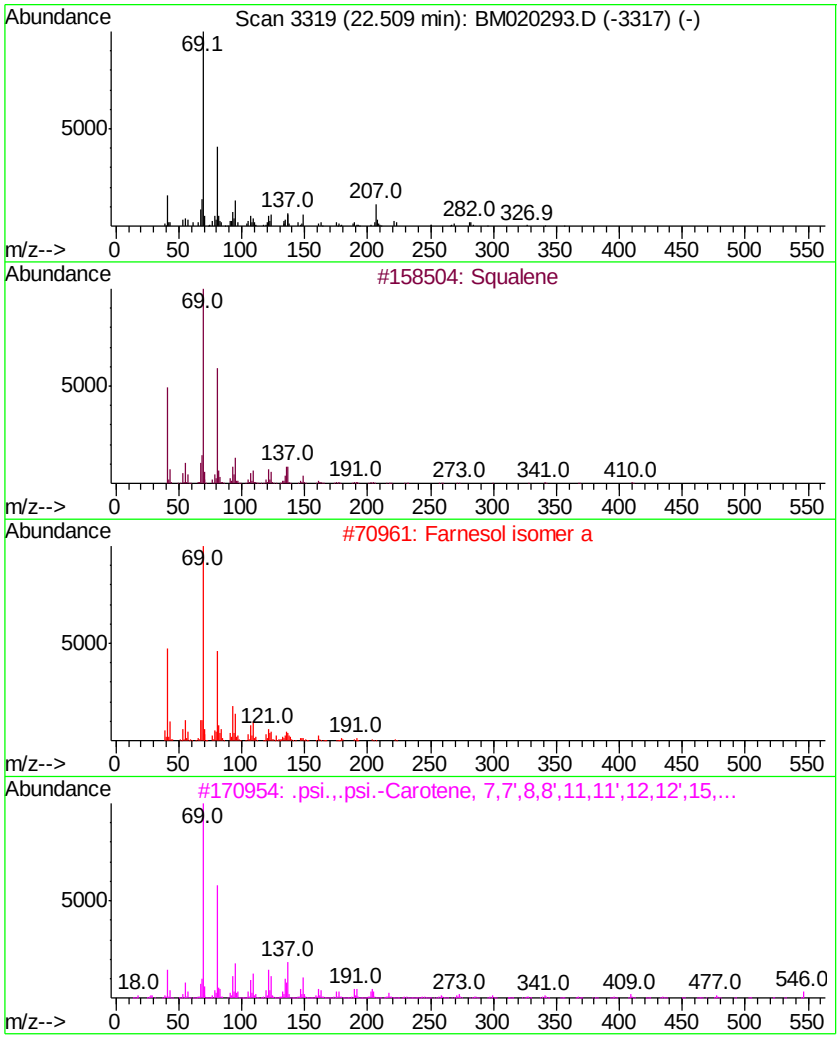
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

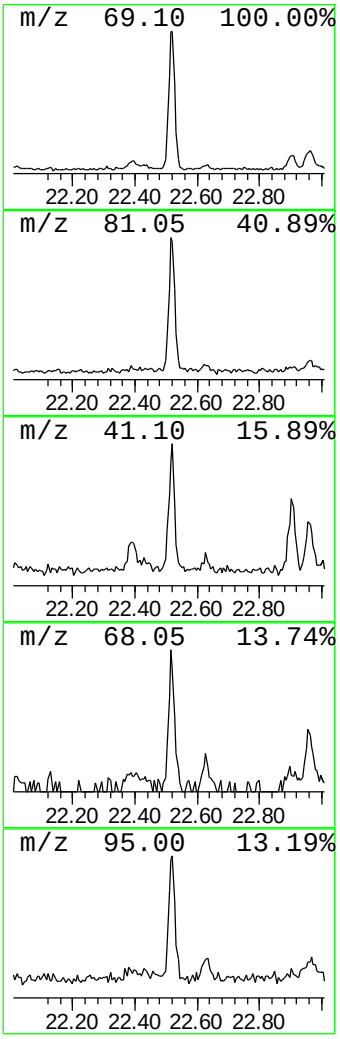
****

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	3.24 ng	158749	Perylene-d12	23.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	81
2	Farnesol isomer a	222	C15H26O	1000108-92-4	72
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	64
4	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	59
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59





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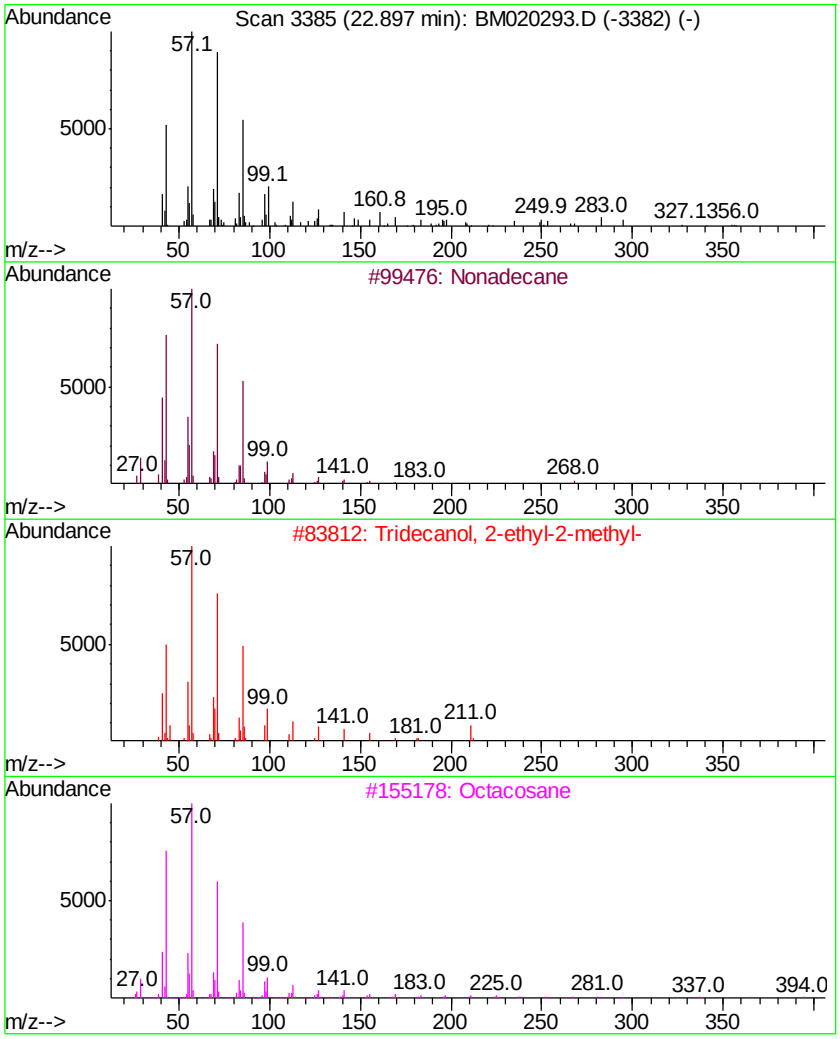
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

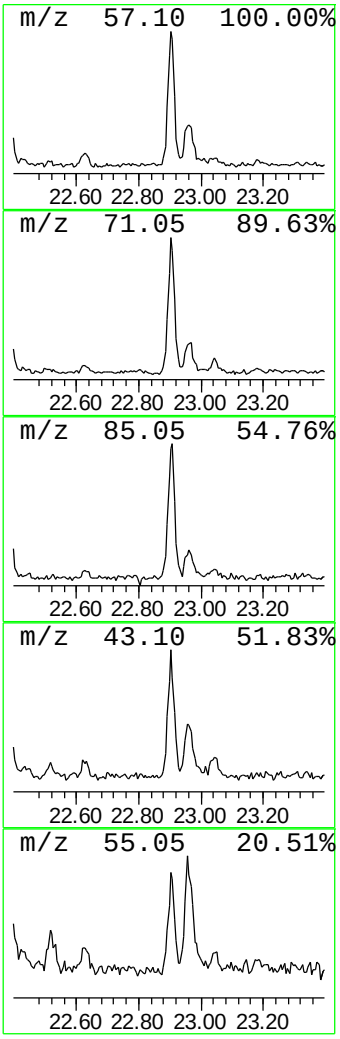
****

Peak Number 7 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.90	2.50 ng	122829	Perylene-d12	23.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	87
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86
3	Octacosane	394	C28H58	000630-02-4	83
4	Triacontane	422	C30H62	000638-68-6	80
5	Nonacosane	408	C29H60	000630-03-5	80





Tentatively Identified Compound (LSC) summary

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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	111.7	ng	1848830	1	7.76	331063	20.0
n-Hexadecanoic acid	18.04	4.0	ng	132239	4	17.16	659506	20.0
Dichloroacetic ac...	21.04	4.0	ng	182807	5	21.35	917029	20.0
unknown21.94	21.94	3.2	ng	147304	5	21.35	917029	20.0
Squalene	22.51	3.2	ng	158749	6	23.63	981066	20.0
Nonadecane	22.90	2.5	ng	122829	6	23.63	981066	20.0