LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

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:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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	5.107	535	539	559	rBV	89015	220284	9.22%	1.178%
2	5.713	638	642	671	rBV	749633	2002838	83.79%	10.714%
3	7.289	906	910	926	rBV	867162	1864319	78.00%	9.973%
4	7.407	926	930	947	rVB	1416694	2390177	100.00%	12.786%
5	7.742	983	987	998	rBV	451860	545877	22.84%	2.920%
6	7.978	1022	1027	1048	rBV	1306457	1661774	69.53%	8.890%
7	8.648	1136	1141	1161	rBV	529819	1157774	48.44%	6.193%
8	9.766	1327	1331	1358	rBV	327655	721331	30.18%	3.859%
9	11.536	1627	1632	1657	rBV	1207295	2107995	88.19%	11.277%
10	12.242	1748	1752	1762	rBV	93474	179107	7.49%	0.958%
11	12.601	1808	1813	1830	rBV2	417175	756469	31.65%	4.047%
12	13.424	1947	1953	1958	rBV	24957	31486	1.32%	0.168%
13	13.901	2029	2034	2051	rBV	475343	930799	38.94%	4.979%
14	14.201	2080	2085	2088	rBV	24672	29177	1.22%	0.156%
15	15.001	2217	2221	2226	rBV	326158	501720	20.99%	2.684%
16	15.954	2379	2383	2401	rVB5	38621	90966	3.81%	0.487%
17	16.789	2521	2525	2536	rBV	123642	171620	7.18%	0.918%
18	17.089	2571	2576	2586	rVB	138725	178245	7.46%	0.954%
19	17.318	2610	2615	2627	rBV	1083201	1340560	56.09%	7.171%
20	17.695	2674	2679	2684	rBV5	17375	25234	1.06%	0.135%
21	18.559	2822	2826	2837	rBV4	39438	80274	3.36%	0.429%
22	18.671	2840	2845	2850	rBV2	436636	640187	26.78%	3.425%
23	18.818	2864	2870	2877	rVB7	23987	48010	2.01%	0.257%
24	19.347	2955	2960	2968	rBV7	15586	40825	1.71%	0.218%
25	19.953	3058	3063	3066	rBV	71262	108930	4.56%	0.583%
26	20.071	3079	3083	3087	rBV4	34116	47206	1.98%	0.253%
27	20.242	3108	3112	3116	rBV	45768	58515	2.45%	0.313%
28	20.300	3119	3122	3126	rVB	56069	67402	2.82%	0.361%
29	20.353	3126	3131	3139	rBV	287164	444158	18.58%	2.376%
30	20.794	3202	3206	3211	rBV2	32368	47582	1.99%	0.255%
31	21.724	3358	3364	3371	rVB8	47915	111162	4.65%	0.595%
32	21.871	3387	3389	3394	rVB5	21574	27818	1.16%	0.149%
33	22.088	3422	3426	3440	rBV4	21043	63764	2.67%	0.341%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

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:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

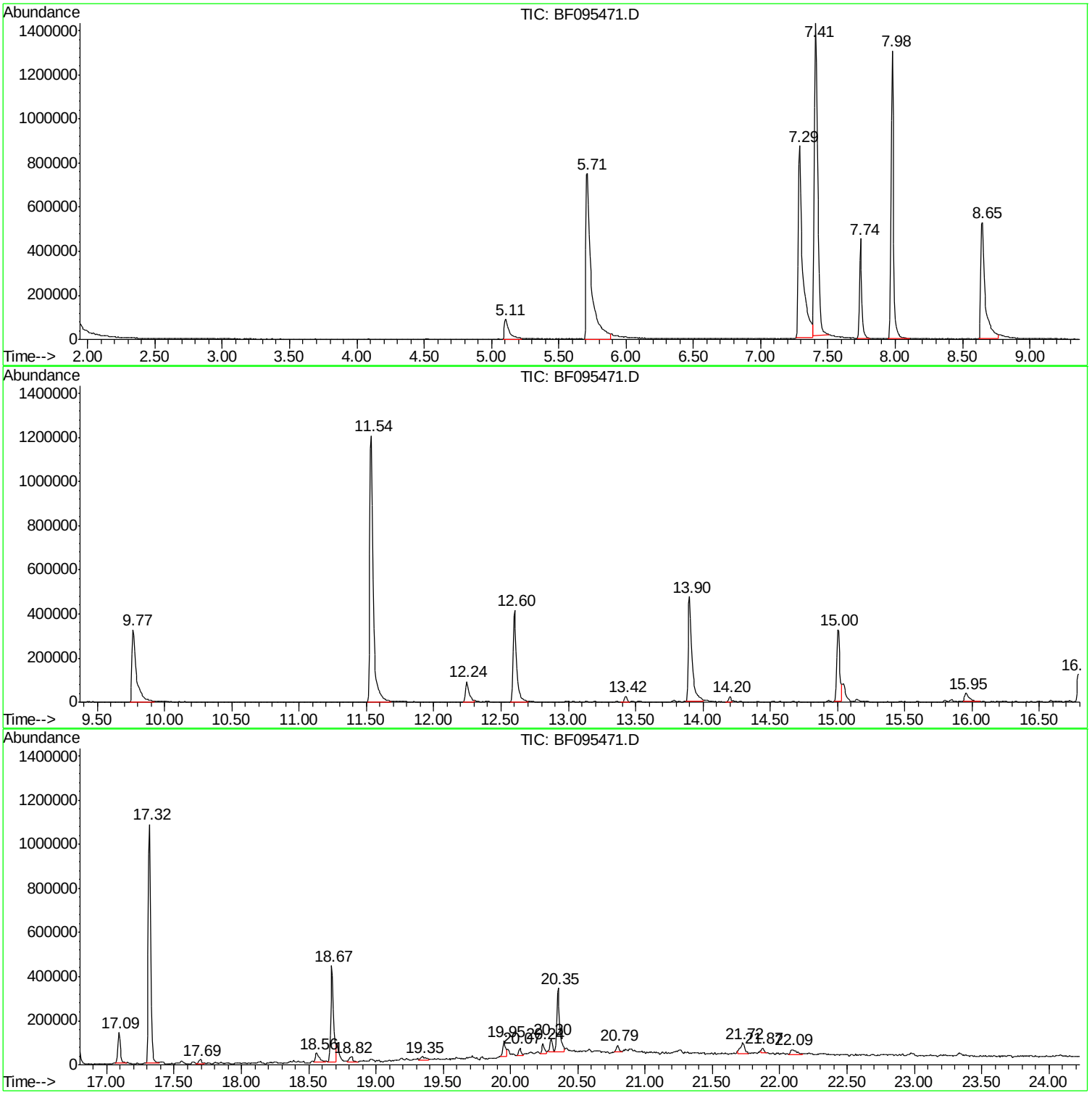
Sum of corrected areas: 18693585

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM3-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

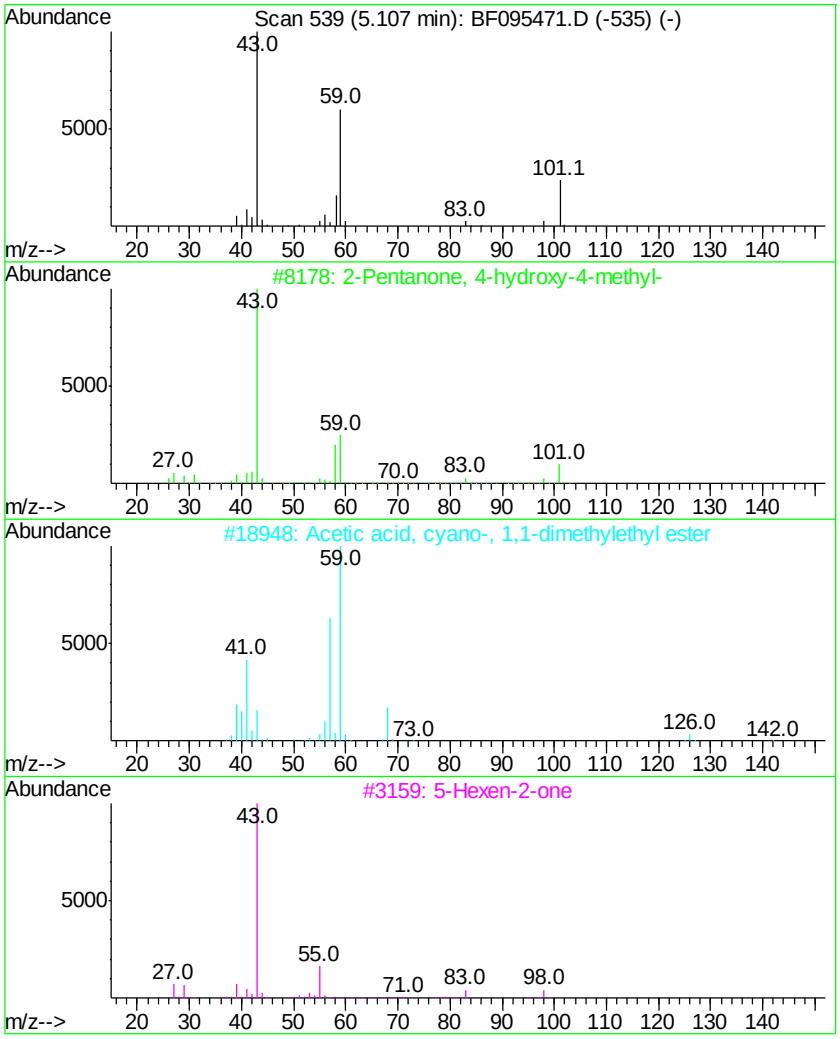
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

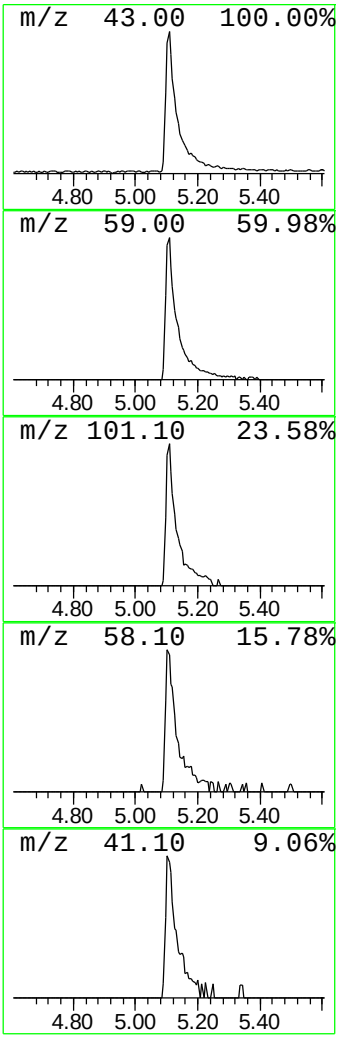
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	8.07 ng	220284	1,4-Dichlorobenzene-d4	7.74

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

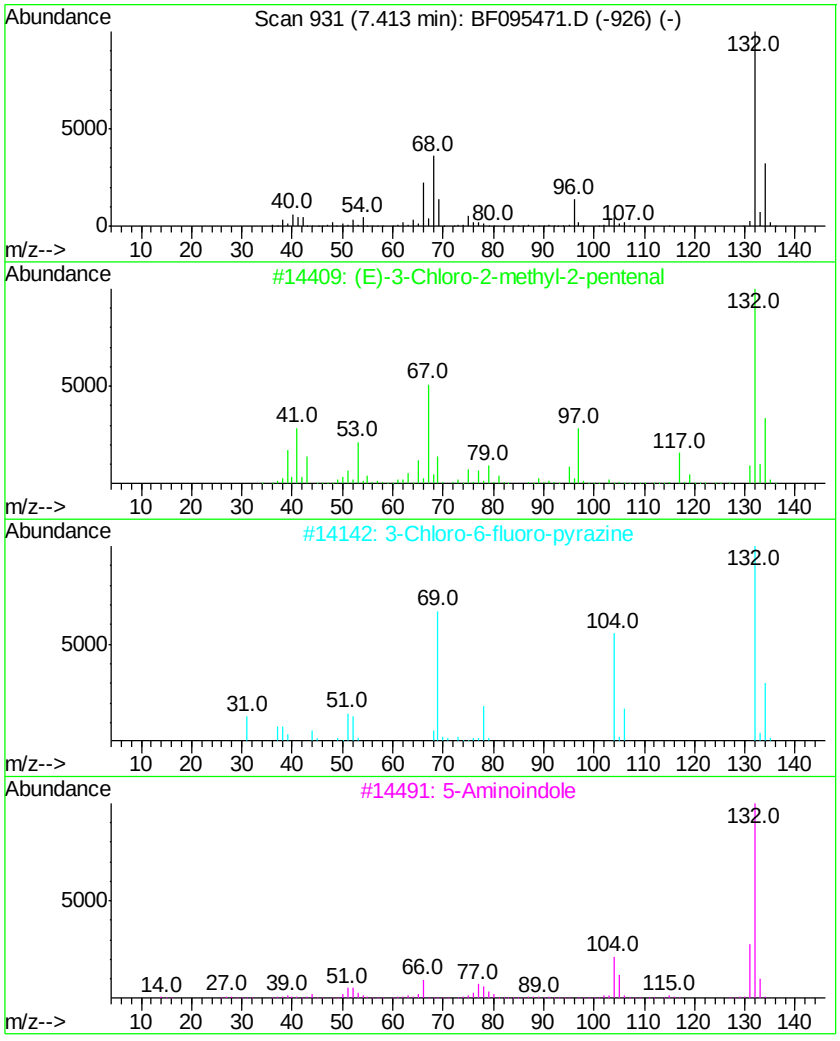
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

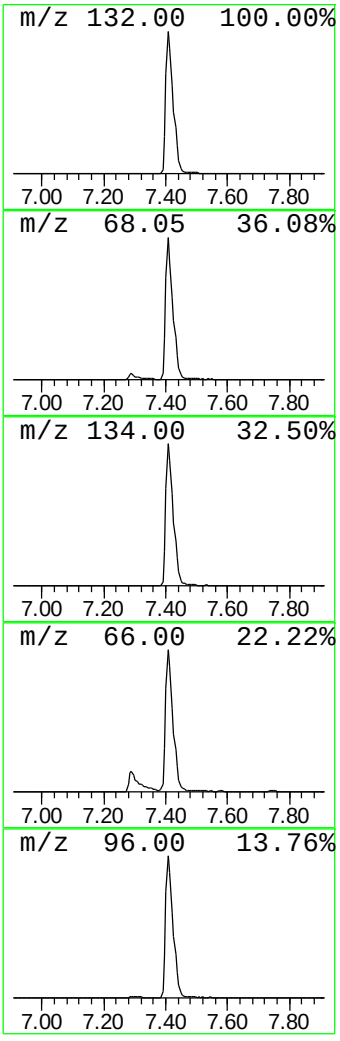
****

Peak Number 2 unknown7.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	87.57 ng	2390180	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

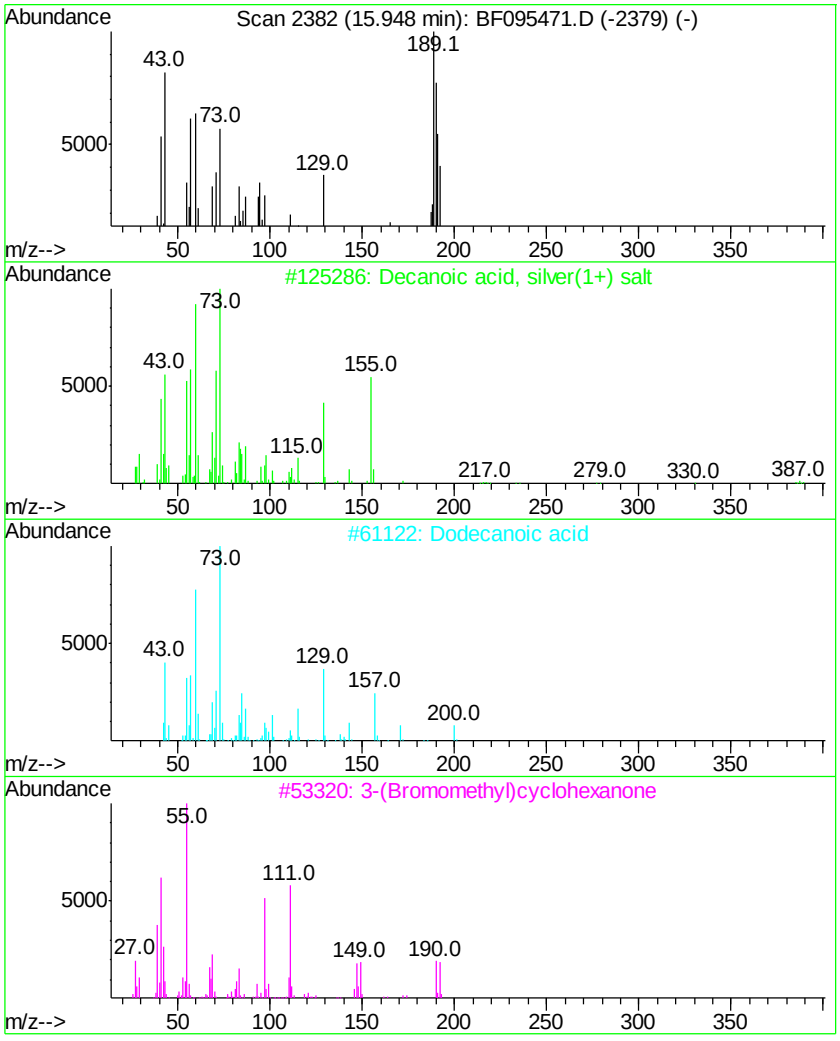
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

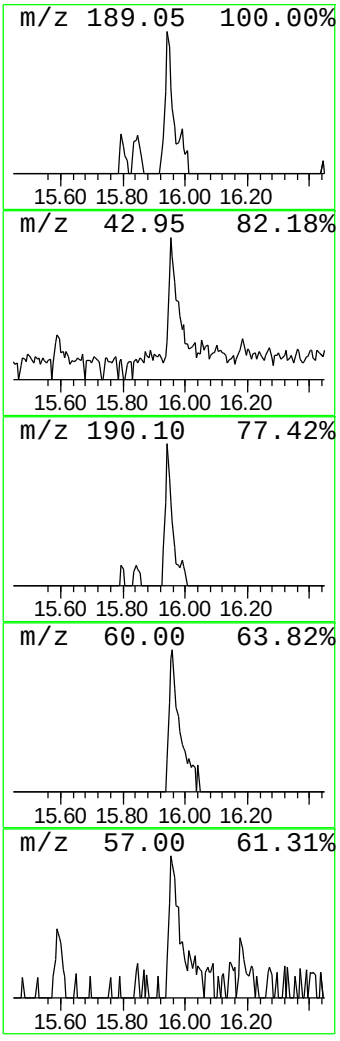
****

Peak Number 4 unknown15.95 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	3.63 ng	90966	Phenanthrene-d10	15.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	14
2	Dodecanoic acid	200	C12H24O2	000143-07-7	10
3	3-(Bromomethyl)cyclohexanone	190	C7H11BrO	168278-83-9	10
4	n-Decanoic acid	172	C10H20O2	000334-48-5	10
5	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

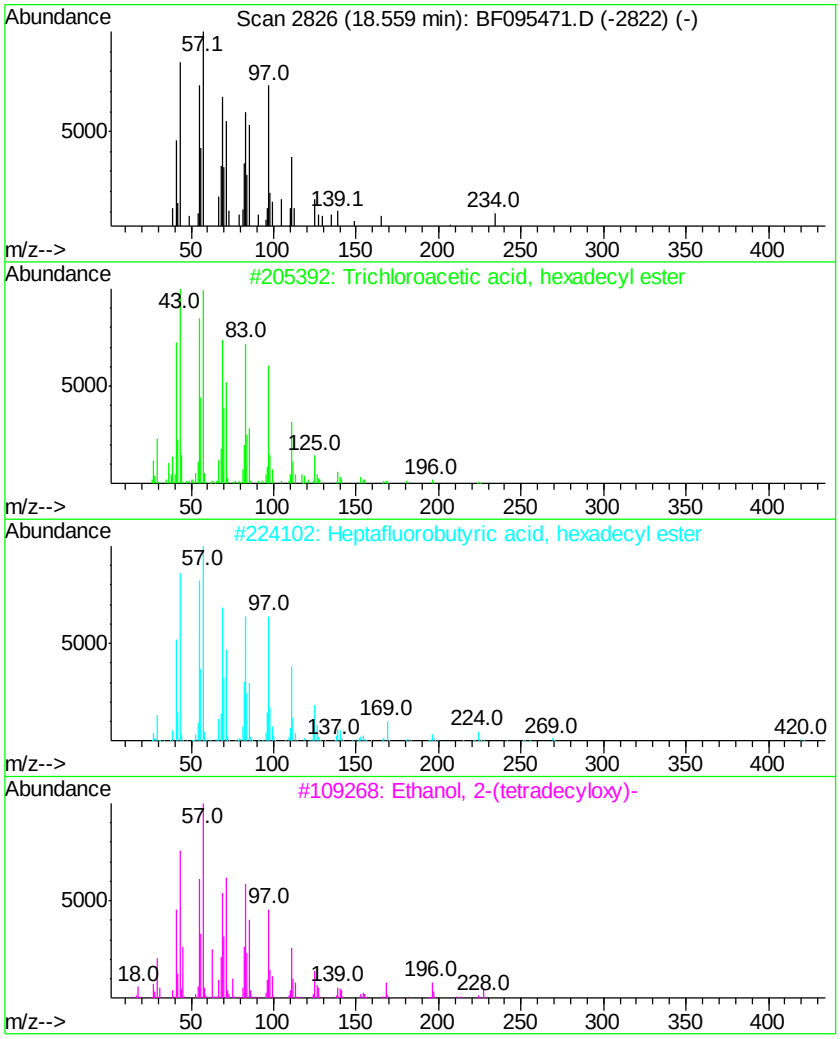
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

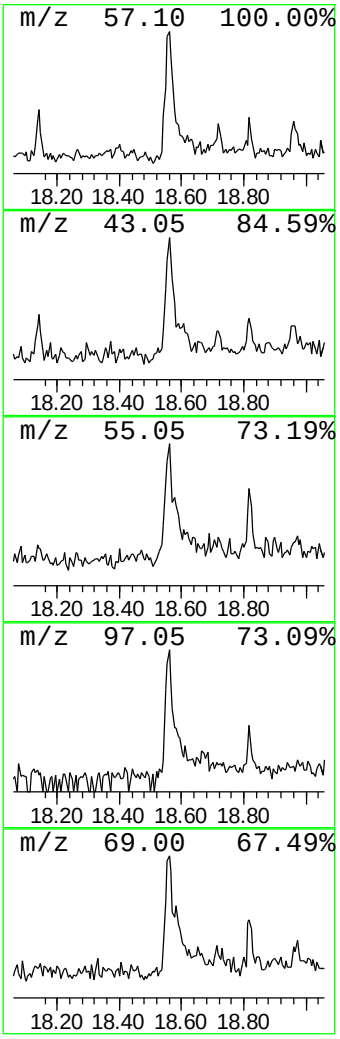
****

Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.56	2.51 ng	80274	Chrysene-d12	18.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

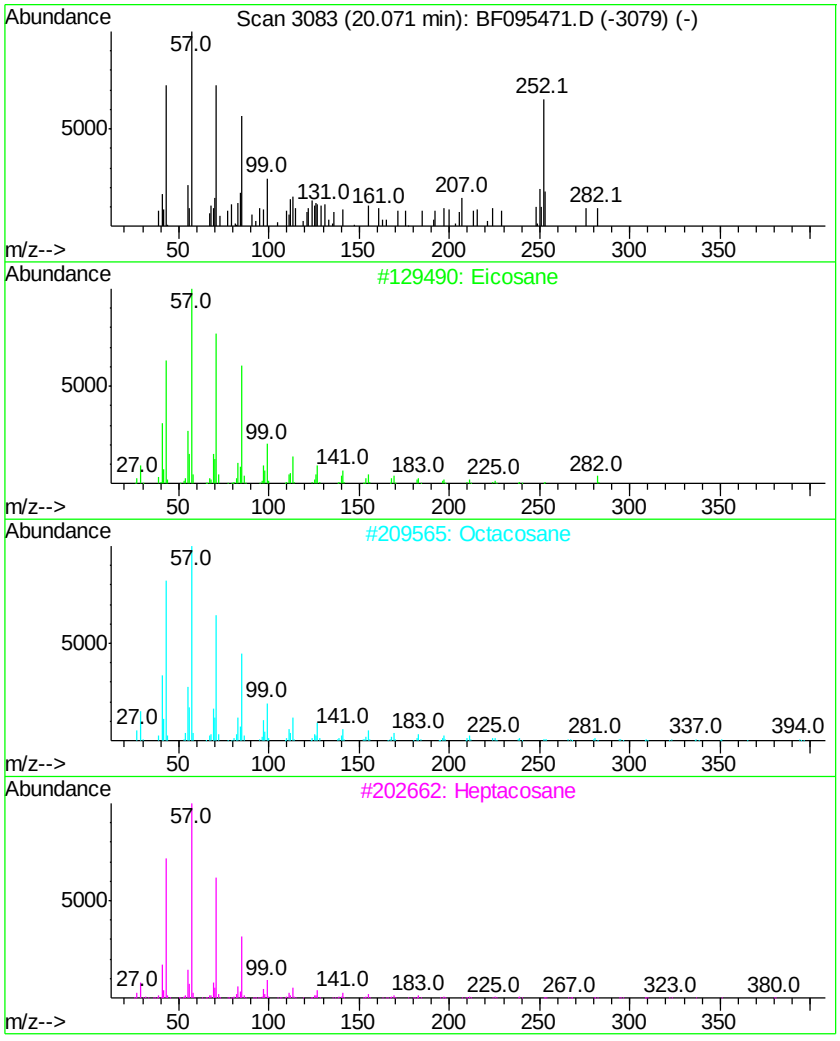
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

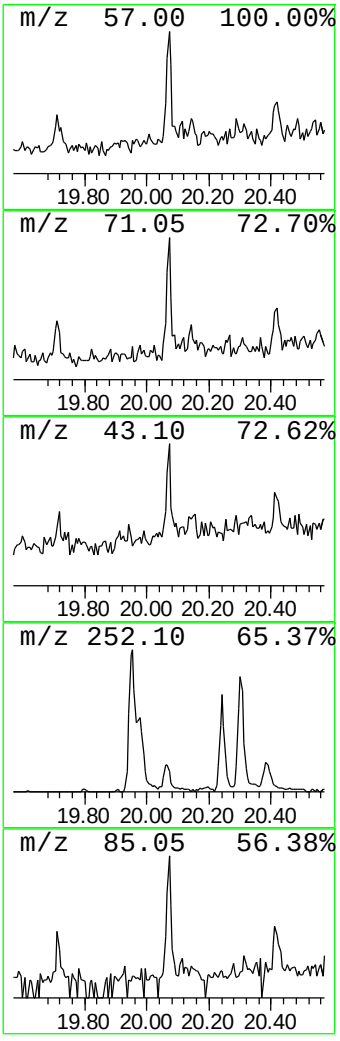
****

Peak Number 6 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	2.13 ng	47206	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	64
2	Octacosane	394	C28H58	000630-02-4	38
3	Heptacosane	380	C27H56	000593-49-7	38
4	Tetracosane	338	C24H50	000646-31-1	38
5	Heneicosane	296	C21H44	000629-94-7	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

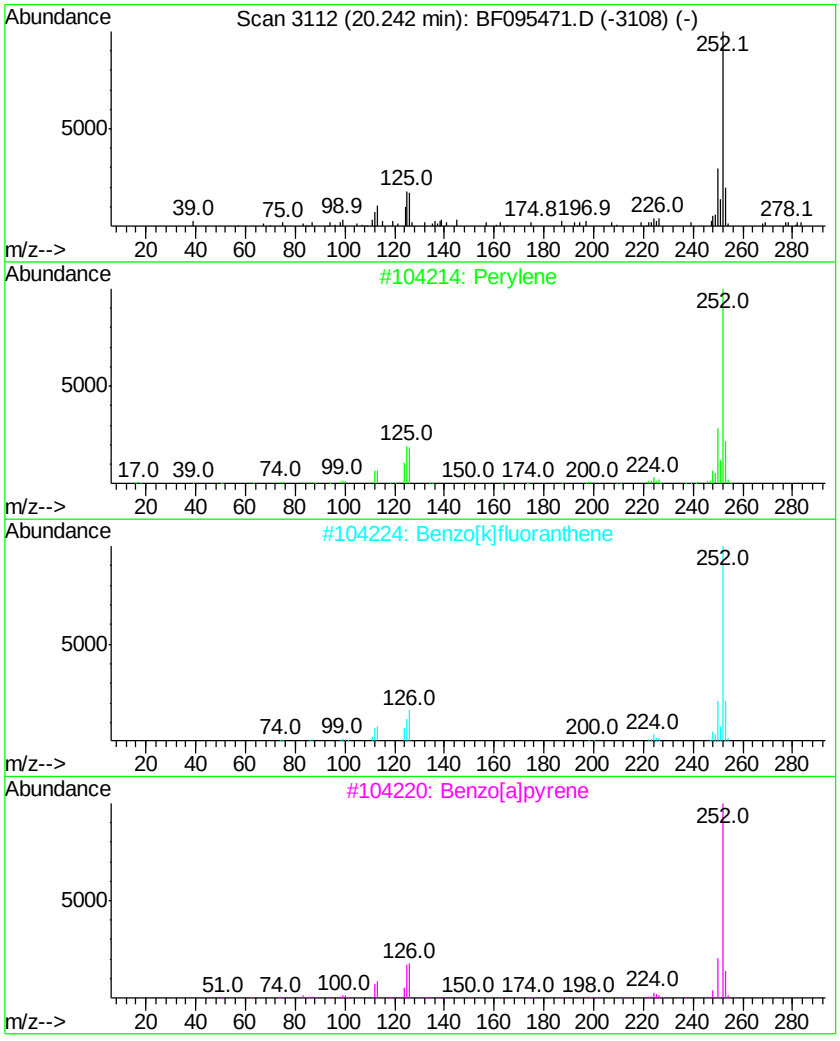
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

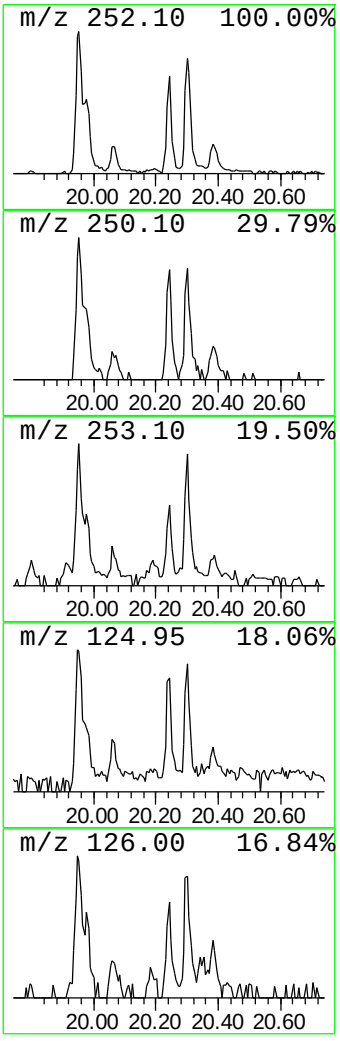
****

Peak Number 7 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.24	2.63 ng	58515	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	93
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[e]pyrene	252	C20H12	000192-97-2	91
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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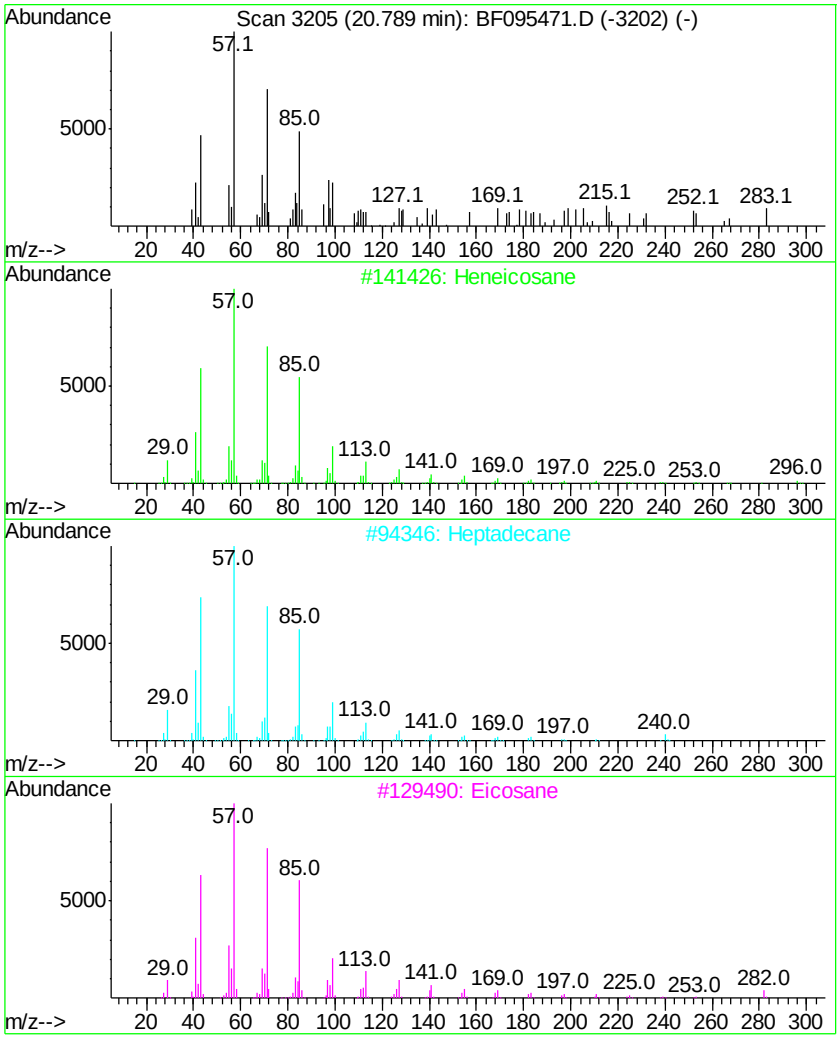
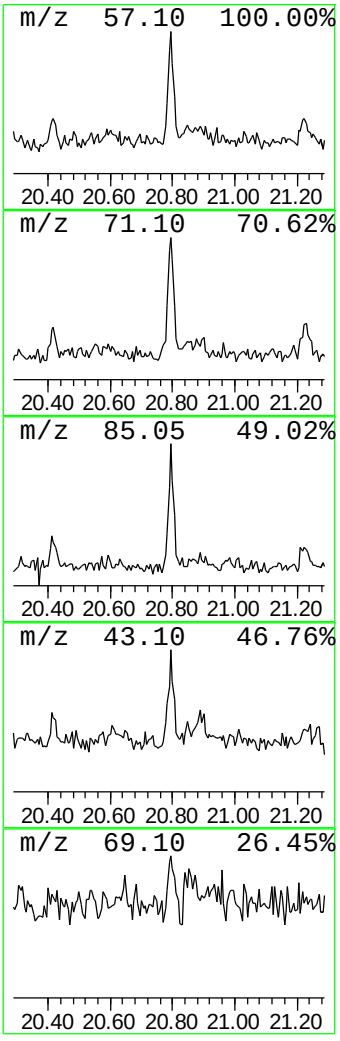
Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	2.14 ng	47582	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Heptadecane	240	C17H36	000629-78-7	80
3	Eicosane	282	C20H42	000112-95-8	72
4	Hentriacontane	437	C31H64	000630-04-6	68
5	Octadecane	254	C18H38	000593-45-3	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

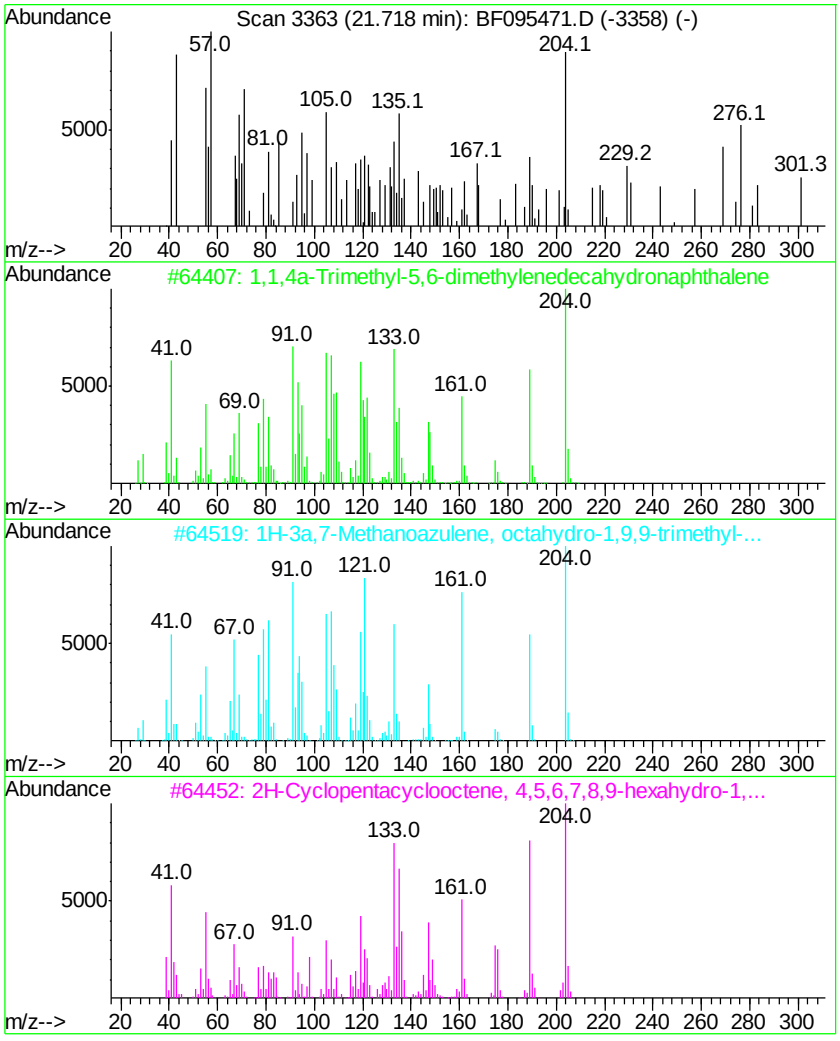
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

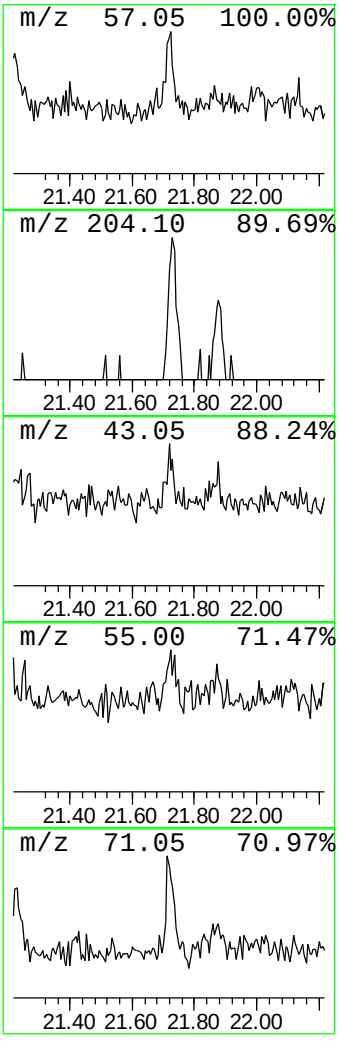
****

Peak Number 9 unknown21.72 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	5.01 ng	111162	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	45
2	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	43
3	2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	41
4	Cyclopropene, 1,3-dimethyl-2,3-b...	204	C7H6F6	054932-73-9	38
5	.delta.-Selinene	204	C15H24	028624-23-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052617\
Data File : BF095471.D
Acq On : 26 May 2017 20:43
Operator : SJ/MA
Sample : I3244-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM3-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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
2-Pentanone, 4-hy...	5.11	8.1	ng	220284	1	7.74	545877	20.0
unknown7.41	7.41	87.6	ng	2390180	1	7.74	545877	20.0
unknown15.95	15.95	3.6	ng	90966	4	15.00	501720	20.0
Trichloroacetic a...	18.56	2.5	ng	80274	5	18.67	640187	20.0
Eicosane	20.07	2.1	ng	47206	6	20.35	444158	20.0
Perylene	20.24	2.6	ng	58515	6	20.35	444158	20.0
Heneicosane	20.79	2.1	ng	47582	6	20.35	444158	20.0
unknown21.72	21.72	5.0	ng	111162	6	20.35	444158	20.0