LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

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-BF022020.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	4.957	485	488	497	rVB	38582	48007	1.39%	0.166%
2	5.369	554	558	575	rBV	2581033	2512988	72.83%	8.666%
3	6.022	666	669	673	rVB	141903	127233	3.69%	0.439%
4	6.386	727	731	740	rBV	2618692	2501313	72.49%	8.626%
5	6.745	788	792	802	rBV	968969	850234	24.64%	2.932%
6	6.898	814	818	822	rBV	2488362	2261577	65.55%	7.799%
7	7.304	883	887	899	rBV	1766269	1694347	49.11%	5.843%
8	8.022	1005	1009	1023	rBV	1192773	1138331	32.99%	3.926%
9	9.098	1187	1192	1196	rBV	3699534	3356950	97.29%	11.577%
10	9.222	1208	1213	1218	rVB	430614	371451	10.77%	1.281%
11	9.492	1253	1259	1263	rBV	166771	147673	4.28%	0.509%
12	9.751	1299	1303	1305	rBV	427717	414479	12.01%	1.429%
13	9.774	1305	1307	1311	rVB	1596560	1310464	37.98%	4.519%
14	10.357	1403	1406	1415	rVB	143027	141390	4.10%	0.488%
15	10.563	1434	1441	1446	rBV	2616484	2441257	70.75%	8.419%
16	11.257	1555	1559	1563	rBV	1682905	1444927	41.88%	4.983%
17	11.486	1594	1598	1607	rBV	58265	64510	1.87%	0.222%
18	11.792	1645	1650	1653	rBV	220631	235566	6.83%	0.812%
19	12.304	1734	1737	1742	rBV	85609	97009	2.81%	0.335%
20	12.504	1768	1771	1775	rVB	39716	37621	1.09%	0.130%
21	12.568	1779	1782	1791	rBV	43024	63162	1.83%	0.218%
22	12.839	1824	1828	1832	rBV	3853262	3450385	100.00%	11.899%
23	13.045	1860	1863	1866	rBV3	35179	41817	1.21%	0.144%
24	13.598	1953	1957	1963	rBV	611024	492367	14.27%	1.698%
25	13.733	1976	1980	1992	rBV	341391	442098	12.81%	1.525%
26	13.892	2003	2007	2018	rVB	1242879	1136720	32.94%	3.920%
27	14.057	2031	2035	2042	rVB	90055	89020	2.58%	0.307%
28	14.362	2083	2087	2096	rBV	171013	199752	5.79%	0.689%
29	14.656	2133	2137	2141	rBV	172216	171055	4.96%	0.590%
30	14.727	2145	2149	2155	rVB	78014	77457	2.24%	0.267%
31	14.974	2186	2191	2199	rBV	210520	247117	7.16%	0.852%
32	15.315	2244	2249	2263	rBV	727639	1062888	30.80%	3.665%
33	15.521	2280	2284	2289	rVB3	39042	50254	1.46%	0.173%
34	15.739	2316	2321	2326	rBV	98330	150862	4.37%	0.520%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

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-BF022020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.792	2326	2330	2339	rVV4	28681	58142	1.69%	0.201%
36	16.209	2396	2401	2406	rBV2	37948	67396	1.95%	0.232%

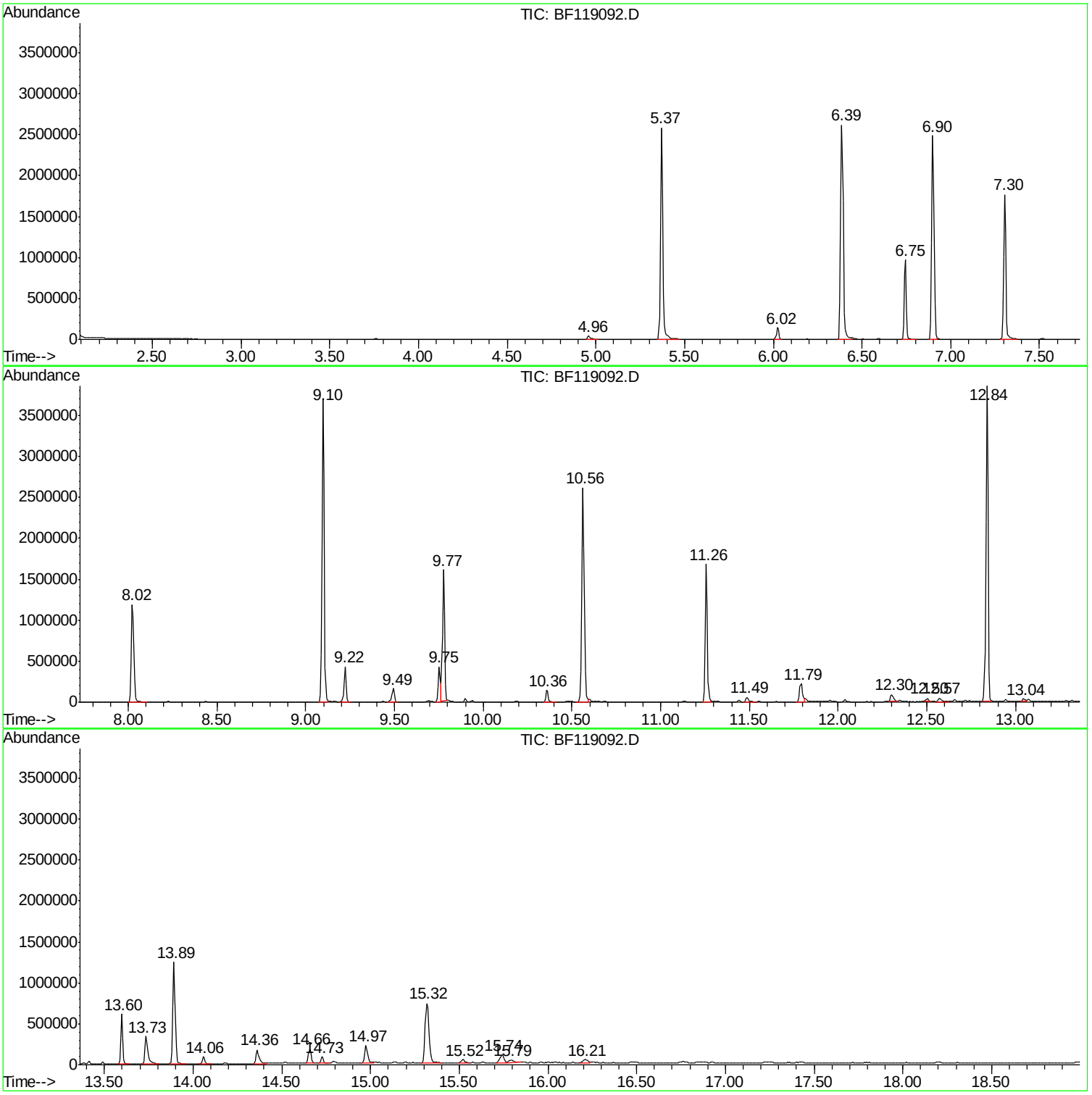
Sum of corrected areas: 28997819

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

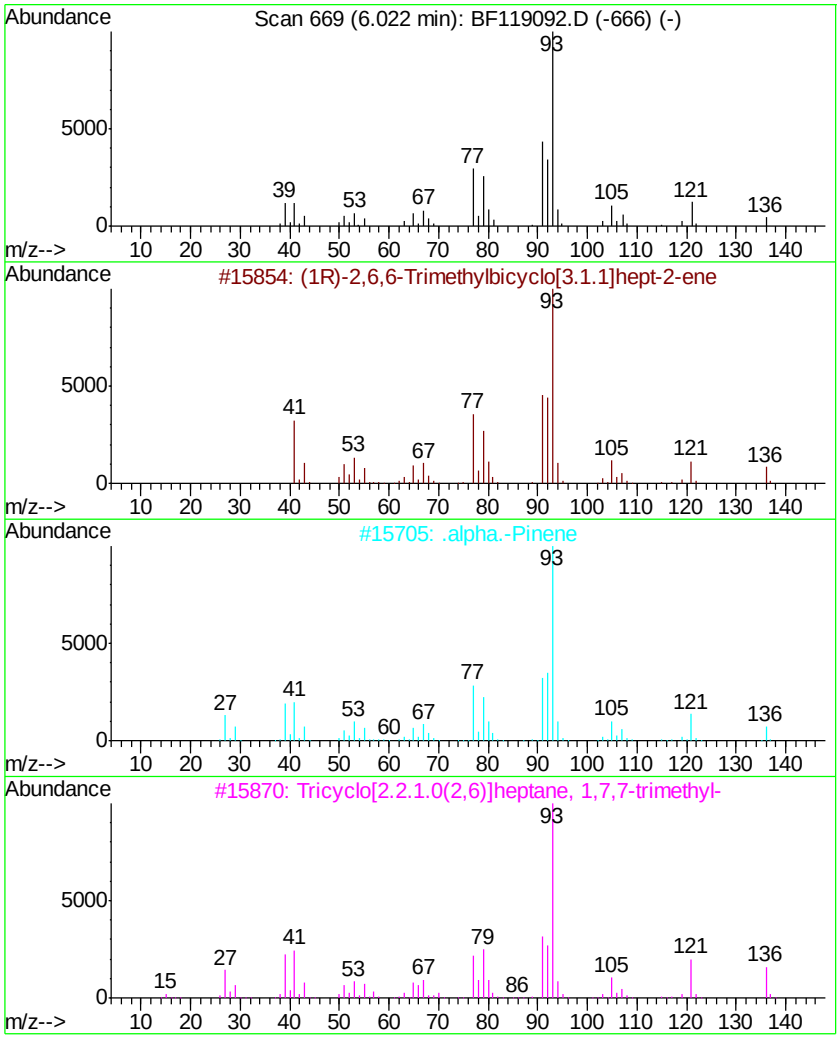
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

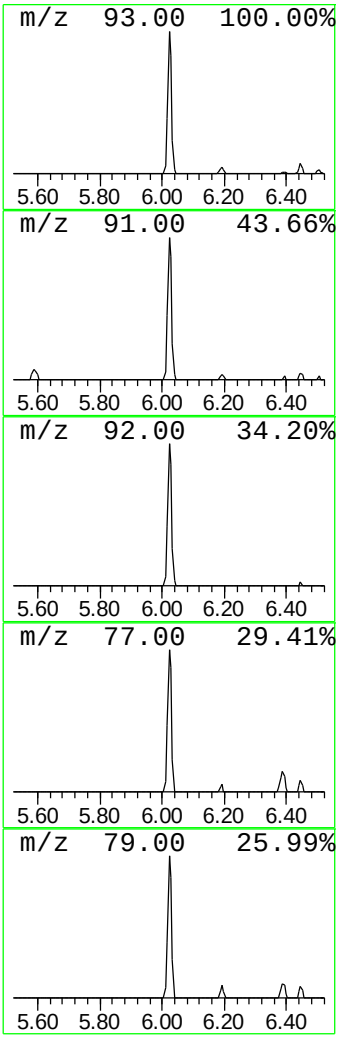
****

Peak Number 1 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.02	2.99 ng	127233	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	95
2	.alpha.-Pinene	136	C10H16	000080-56-8	94
3	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4	(+)-3-Carene	136	C10H16	000498-15-7	90
5	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

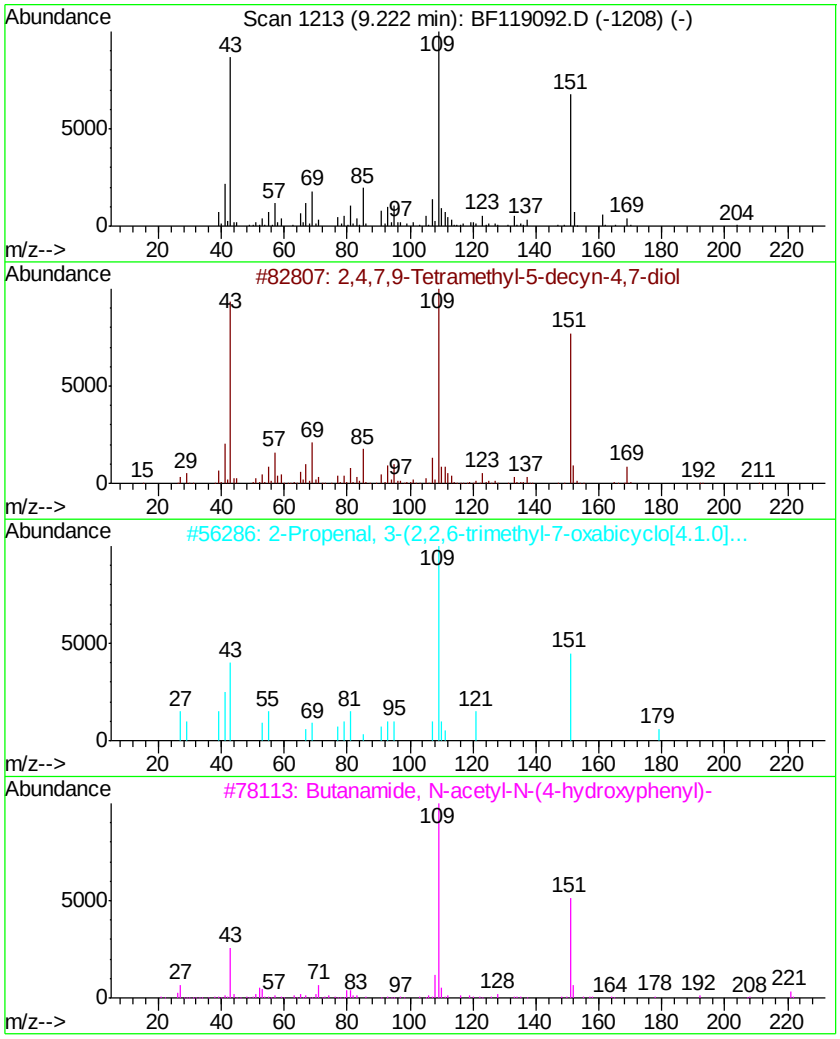
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

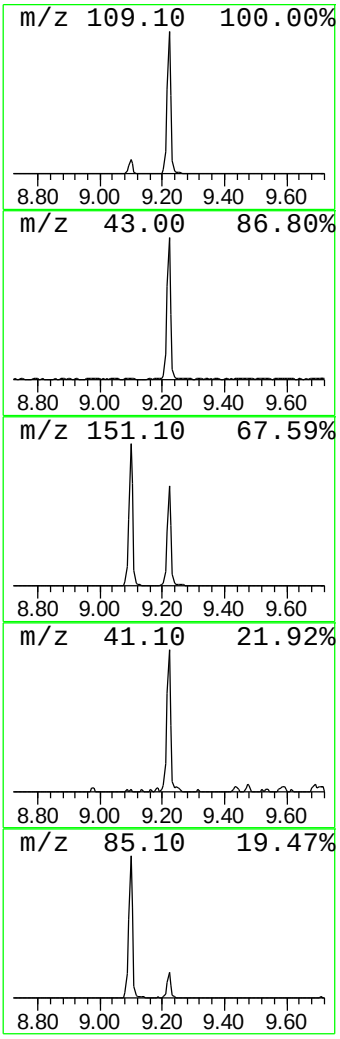
****

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.22	5.67 ng	371451	Acenaphthene-d10	9.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	59
3	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	50
4	Metacetamol	151	C8H9NO2	000621-42-1	50
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

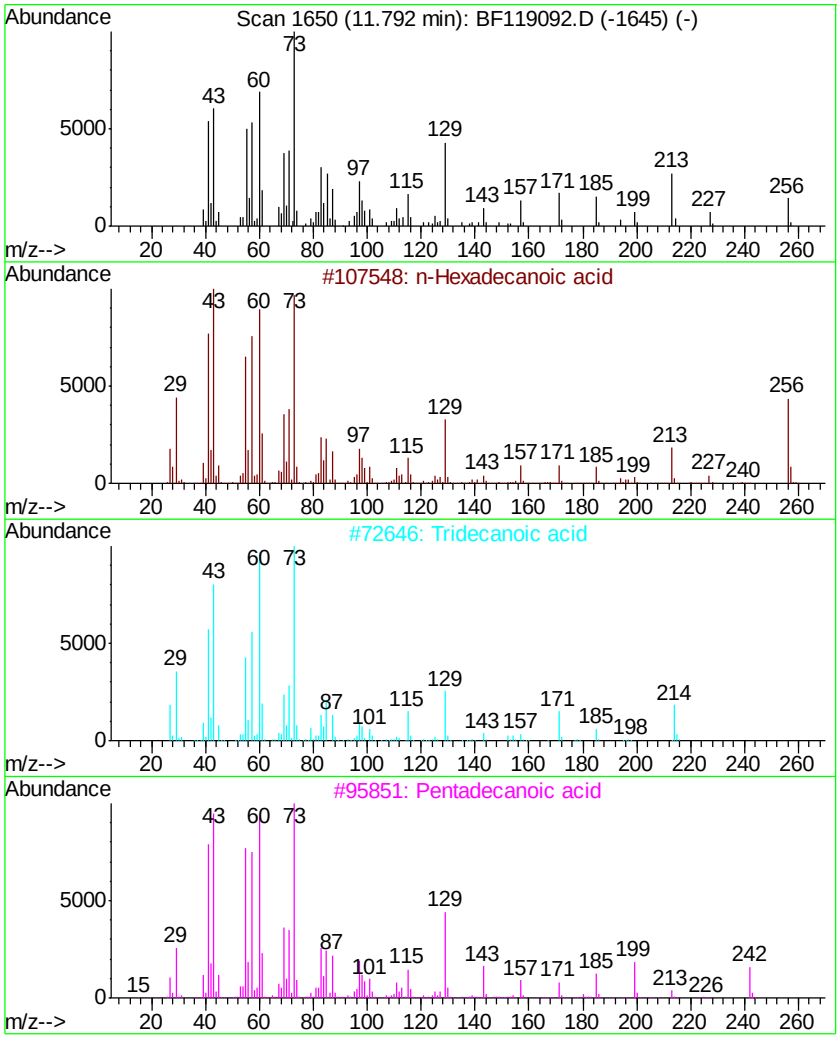
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

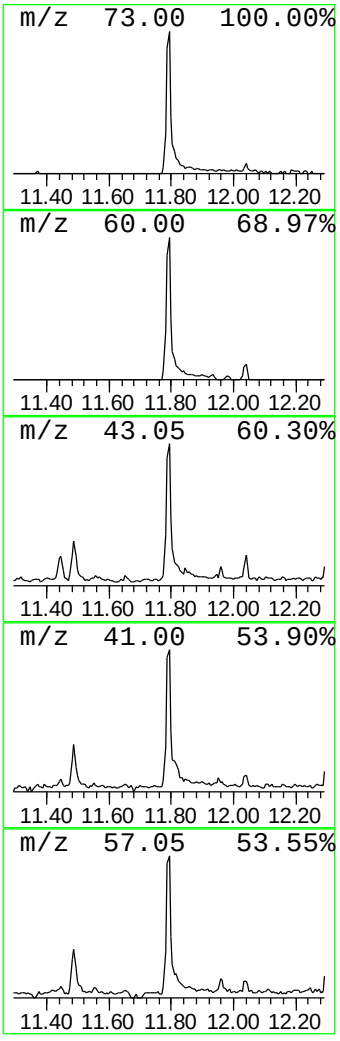
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	3.26 ng	235566	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

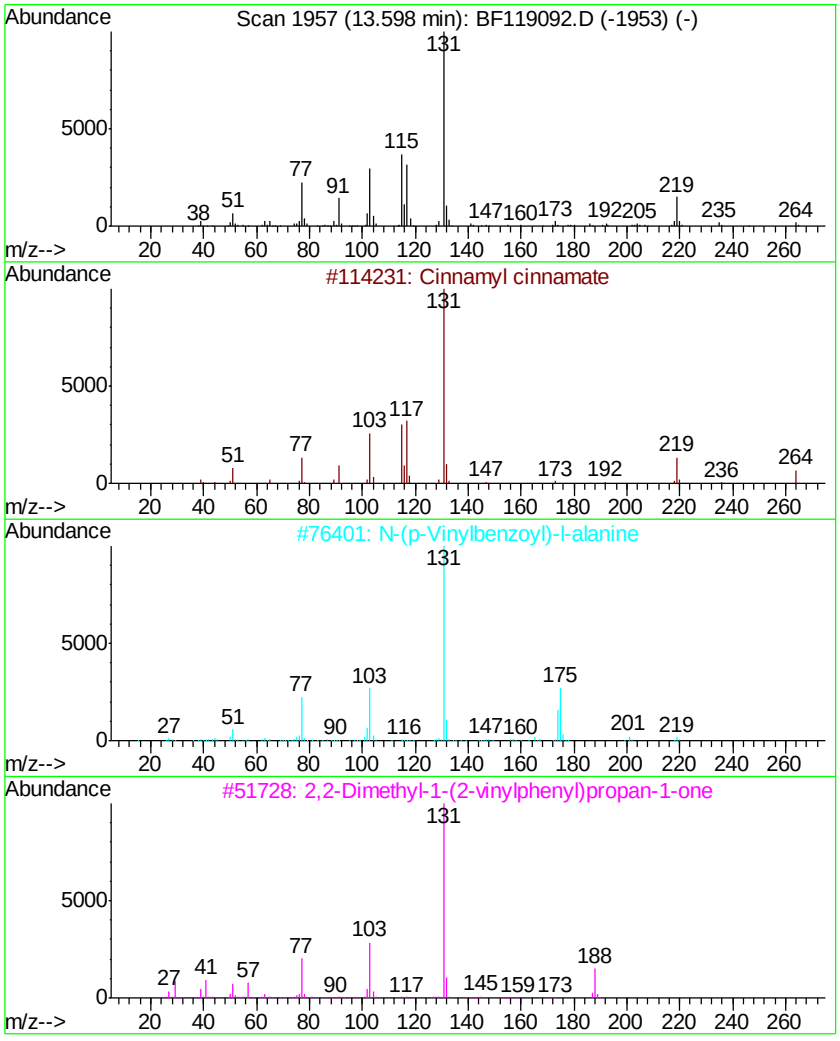
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

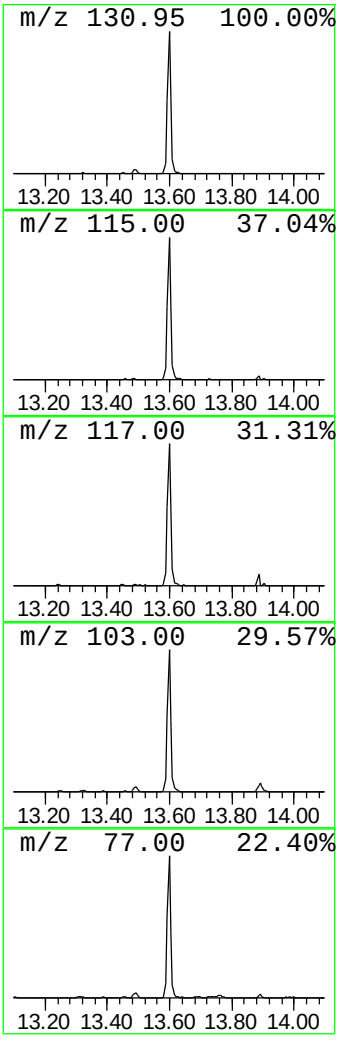
****

Peak Number 6 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	8.66 ng	492367	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	87
2	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	50
3	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	50
4	2-Propenamide, N-(1-methylethyl)...	265	C18H19NO	055044-37-6	50
5	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

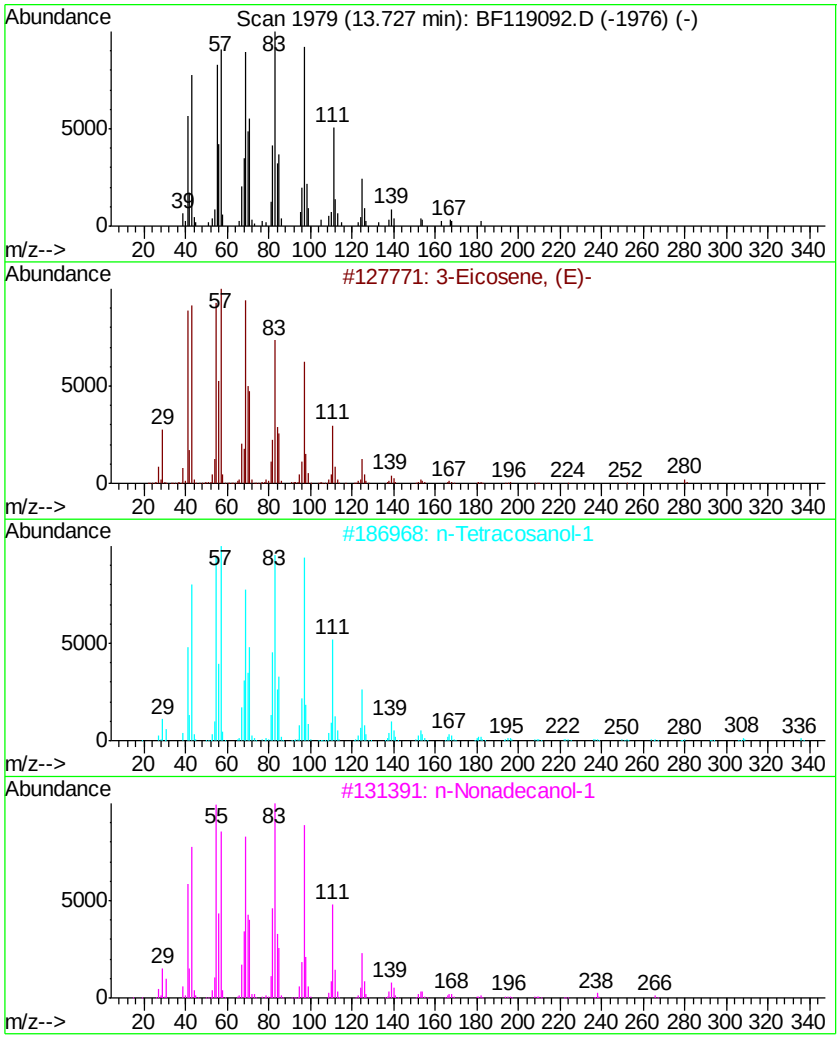
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

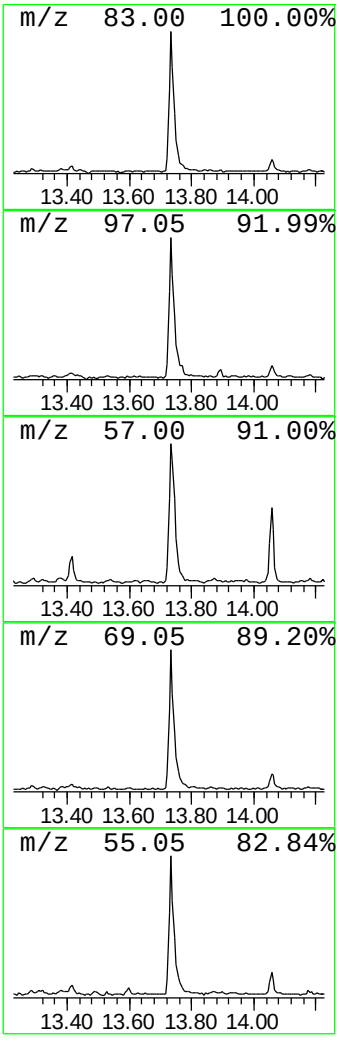
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.78 ng	442098	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	99
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

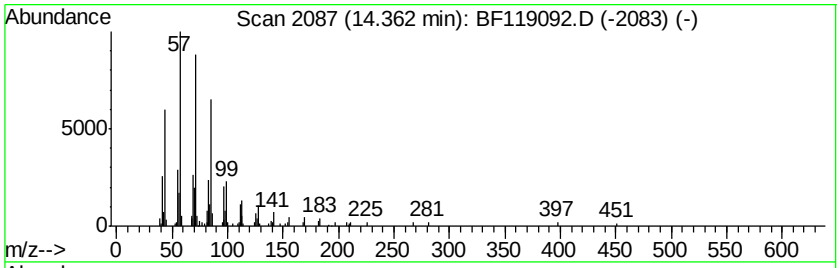
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

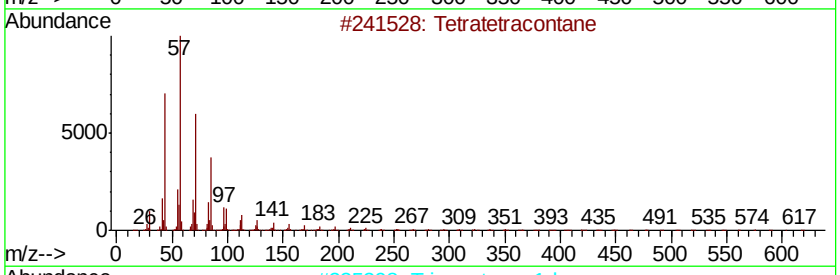
****

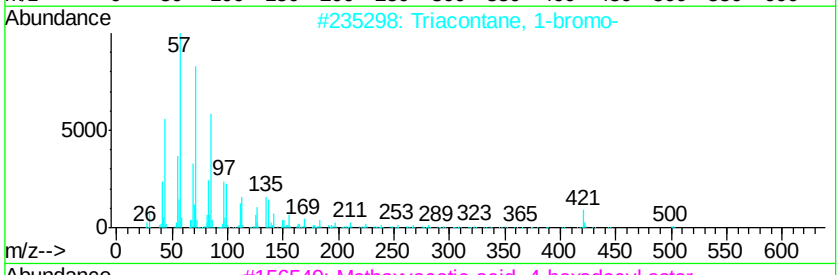
Peak Number 8 Tetratetracontane Concentration Rank 6

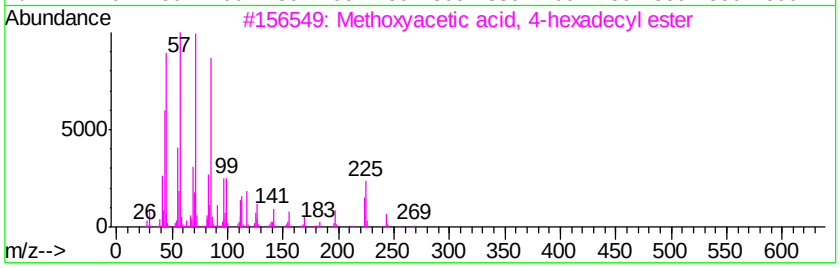
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	3.51 ng	199752	Chrysene-d12	13.89

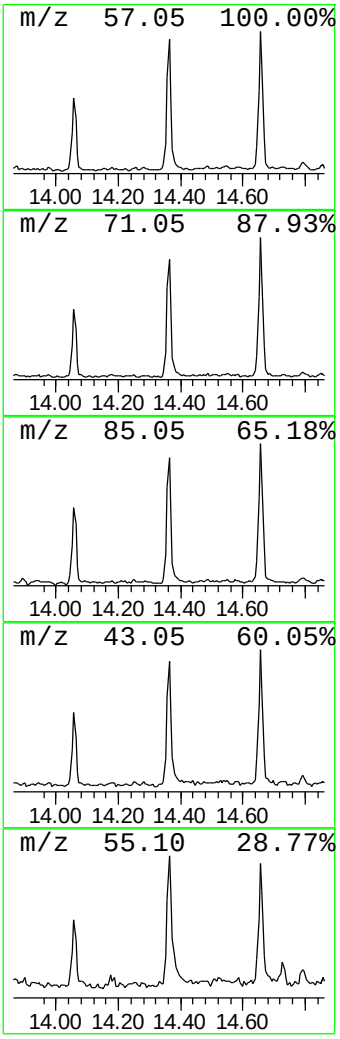
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Triacontane, 1-bromo-	500	C30H61Br	004209-22-7	91
3	Methoxyacetic acid, 4-hexadecyl ...	314	C19H38O3	1000282-99-0	91
4	2-methylhexacosane	380	C27H56	1000376-72-7	91
5	Heptacosane	380	C27H56	000593-49-7	91











Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

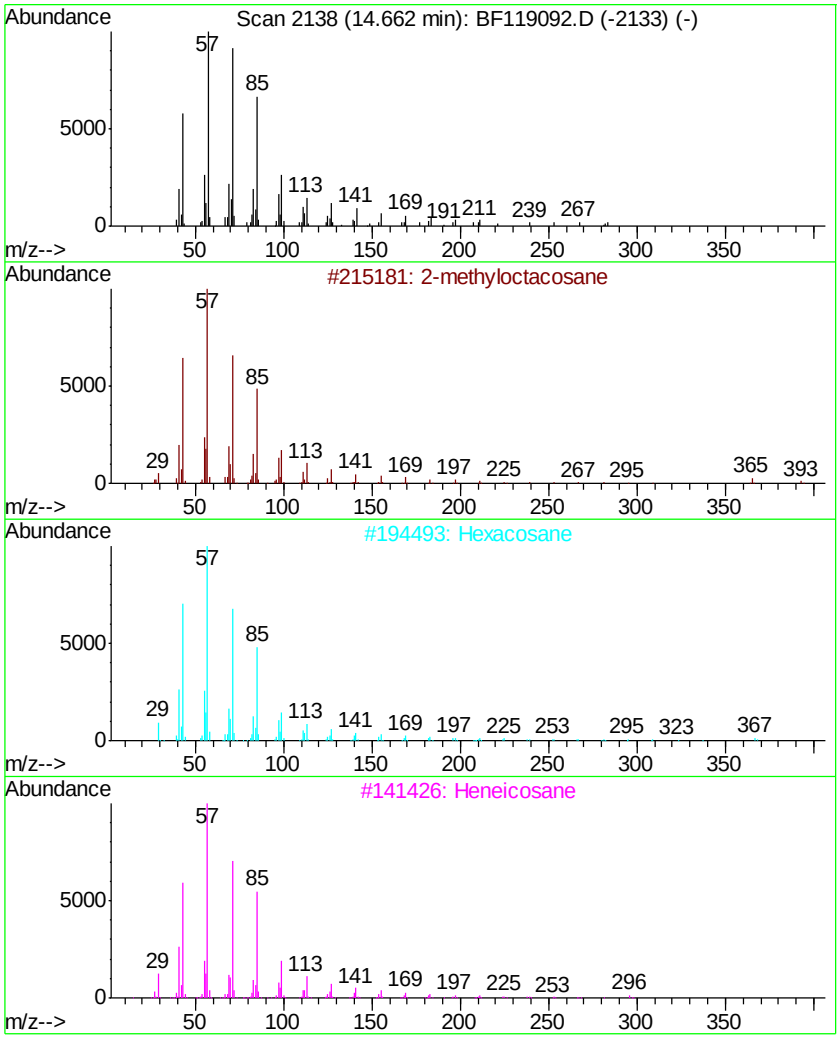
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

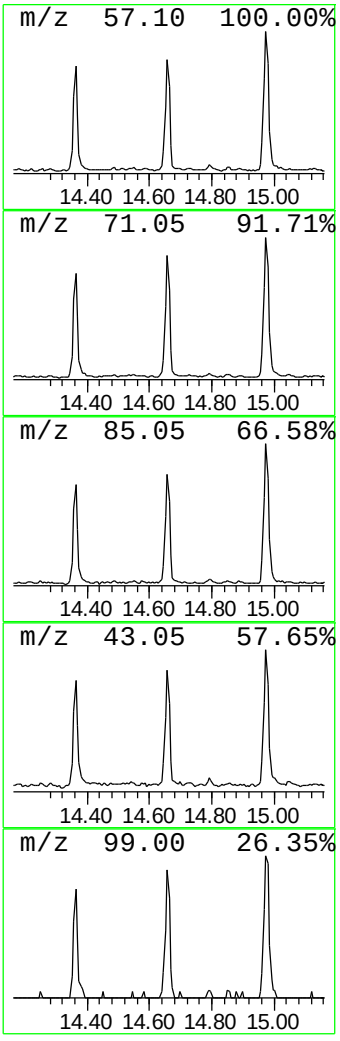
****

Peak Number 9 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.22 ng	171055	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Triacontane	422	C30H62	000638-68-6	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

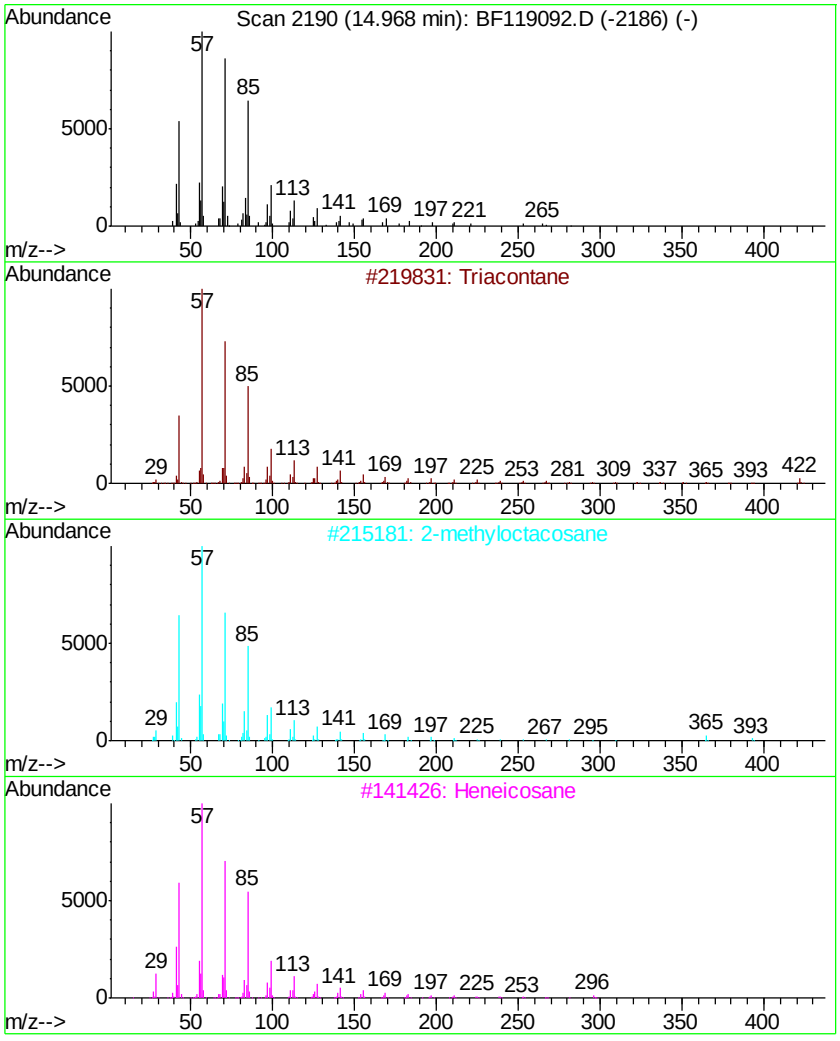
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

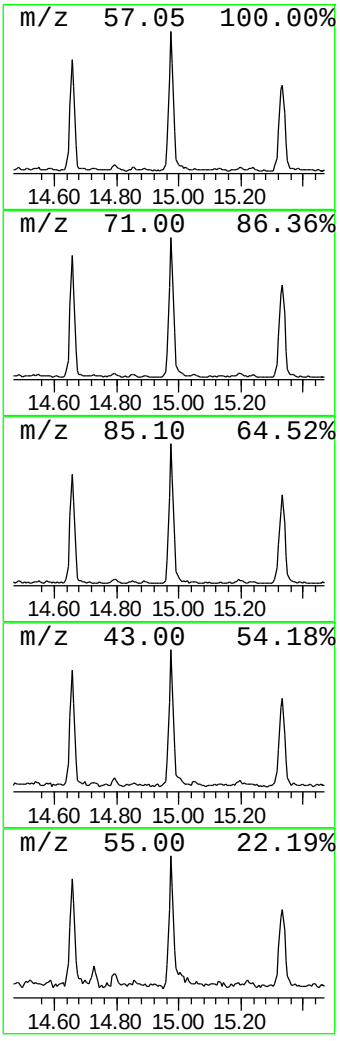
****

Peak Number 10 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	4.65 ng	247117	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5	Octacosane	394	C28H58	000630-02-4	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

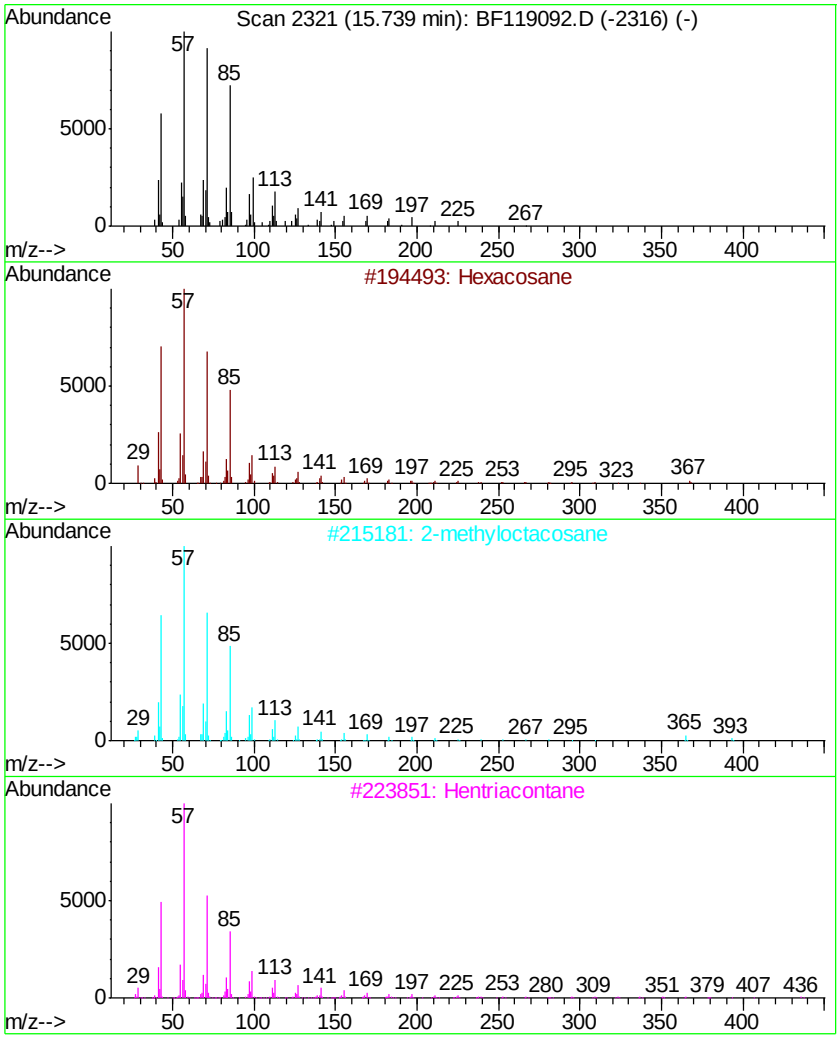
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

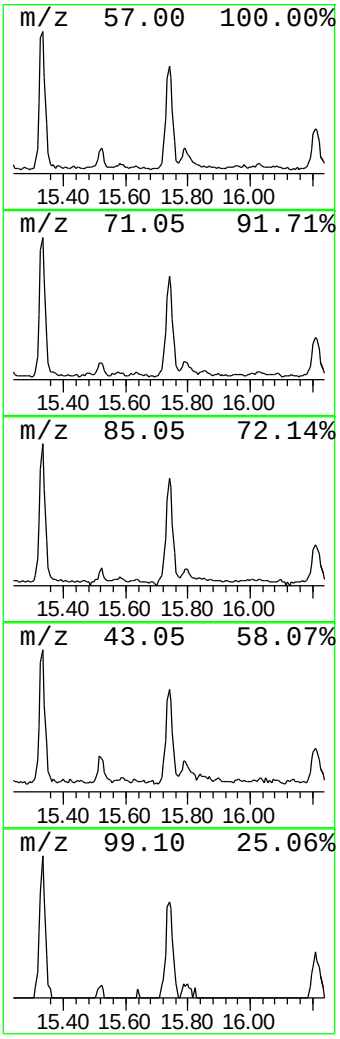
****

Peak Number 11 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.84 ng	150862	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Heptacosane	380	C27H56	000593-49-7	87
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022620\
Data File : BF119092.D
Acq On : 26 Feb 2020 13:55
Operator : CG/JU
Sample : L1681-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SH-BORING-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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
(1R)-2,6,6-Trimet...	6.02	3.0	ng	127233	1	6.75	850234	20.0
2,4,7,9-Tetrameth...	9.22	5.7	ng	371451	3	9.77	1310460	20.0
n-Hexadecanoic acid	11.79	3.3	ng	235566	4	11.26	1444930	20.0
Cinnamyl cinnamate	13.60	8.7	ng	492367	5	13.89	1136720	20.0
3-Eicosene, (E)-	13.73	7.8	ng	442098	5	13.89	1136720	20.0
Tetratetracontane	14.36	3.5	ng	199752	5	13.89	1136720	20.0
2-methyloctacosane	14.66	3.2	ng	171055	6	15.32	1062890	20.0
Triacontane	14.97	4.7	ng	247117	6	15.32	1062890	20.0
Hexacosane	15.74	2.8	ng	150862	6	15.32	1062890	20.0