LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
Data File : BP000551.D
Acq On : 07 Oct 2019 18:32
Operator : JU
Sample : K5213-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

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_P\METHODS\8270-BP100119.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	5.387	556	561	564	rBV	5265395	4867401	64.52%	7.927%
2	6.404	729	734	749	rBV	5290018	5392031	71.48%	8.781%
3	6.534	752	756	759	rBV	6430398	5415279	71.79%	8.819%
4	6.763	791	795	798	rBV	1780582	1513469	20.06%	2.465%
5	6.916	817	821	825	rBV	5506927	4601573	61.00%	7.494%
6	7.322	886	890	893	rBV	3872962	3172365	42.05%	5.166%
7	8.046	1009	1013	1016	rBV	2370875	1912379	25.35%	3.114%
8	9.128	1193	1197	1200	rBV	8231119	6847562	90.77%	11.152%
9	9.210	1207	1211	1215	rBV5	48069	82211	1.09%	0.134%
10	9.245	1215	1217	1220	rVV	91948	84756	1.12%	0.138%
11	9.522	1261	1264	1269	rBV	1366574	1077545	14.28%	1.755%
12	9.804	1307	1312	1316	rBV	2742970	2423071	32.12%	3.946%
13	10.604	1443	1448	1451	rBV	4664677	4202299	55.71%	6.844%
14	10.740	1467	1471	1477	rVB2	89255	136143	1.80%	0.222%
15	11.304	1563	1567	1570	rBV	2948938	2485670	32.95%	4.048%
16	11.375	1576	1579	1583	rVB2	206087	176306	2.34%	0.287%
17	11.545	1605	1608	1617	rBV6	60627	114791	1.52%	0.187%
18	11.845	1656	1659	1663	rBV2	173604	177198	2.35%	0.289%
19	12.369	1745	1748	1755	rBV	241710	407330	5.40%	0.663%
20	12.528	1772	1775	1778	rBV	298396	259912	3.45%	0.423%
21	12.757	1810	1814	1817	rBV	289663	276082	3.66%	0.450%
22	12.910	1836	1840	1843	rBV	8290214	7543569	100.00%	12.285%
23	13.157	1876	1882	1885	rBV4	123857	180380	2.39%	0.294%
24	13.504	1938	1941	1943	rBV	98694	91106	1.21%	0.148%
25	13.828	1993	1996	2007	rVB	541915	799092	10.59%	1.301%
26	13.975	2016	2021	2024	rBV	2791959	2619090	34.72%	4.265%
27	14.157	2049	2052	2056	rBV	159355	149049	1.98%	0.243%
28	14.463	2101	2104	2107	rBV	230457	206801	2.74%	0.337%
29	14.775	2154	2157	2165	rVB	234338	258760	3.43%	0.421%
30	14.851	2166	2170	2175	rVV	462234	473680	6.28%	0.771%
31	15.022	2196	2199	2207	rVB	154778	280550	3.72%	0.457%
32	15.116	2212	2215	2220	rVB2	219332	271233	3.60%	0.442%
33	15.322	2248	2250	2257	rVB	118794	146351	1.94%	0.238%
34	15.386	2258	2261	2267	rBV	134750	157229	2.08%	0.256%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
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Acq On : 07 Oct 2019 18:32
Operator : JU
Sample : K5213-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

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_P\METHODS\8270-BP100119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.451	2267	2272	2277	rBV	1995297	2450757	32.49%	3.991%
36	15.939	2352	2355	2360	rBV	106555	150466	1.99%	0.245%

Sum of corrected areas: 61403486

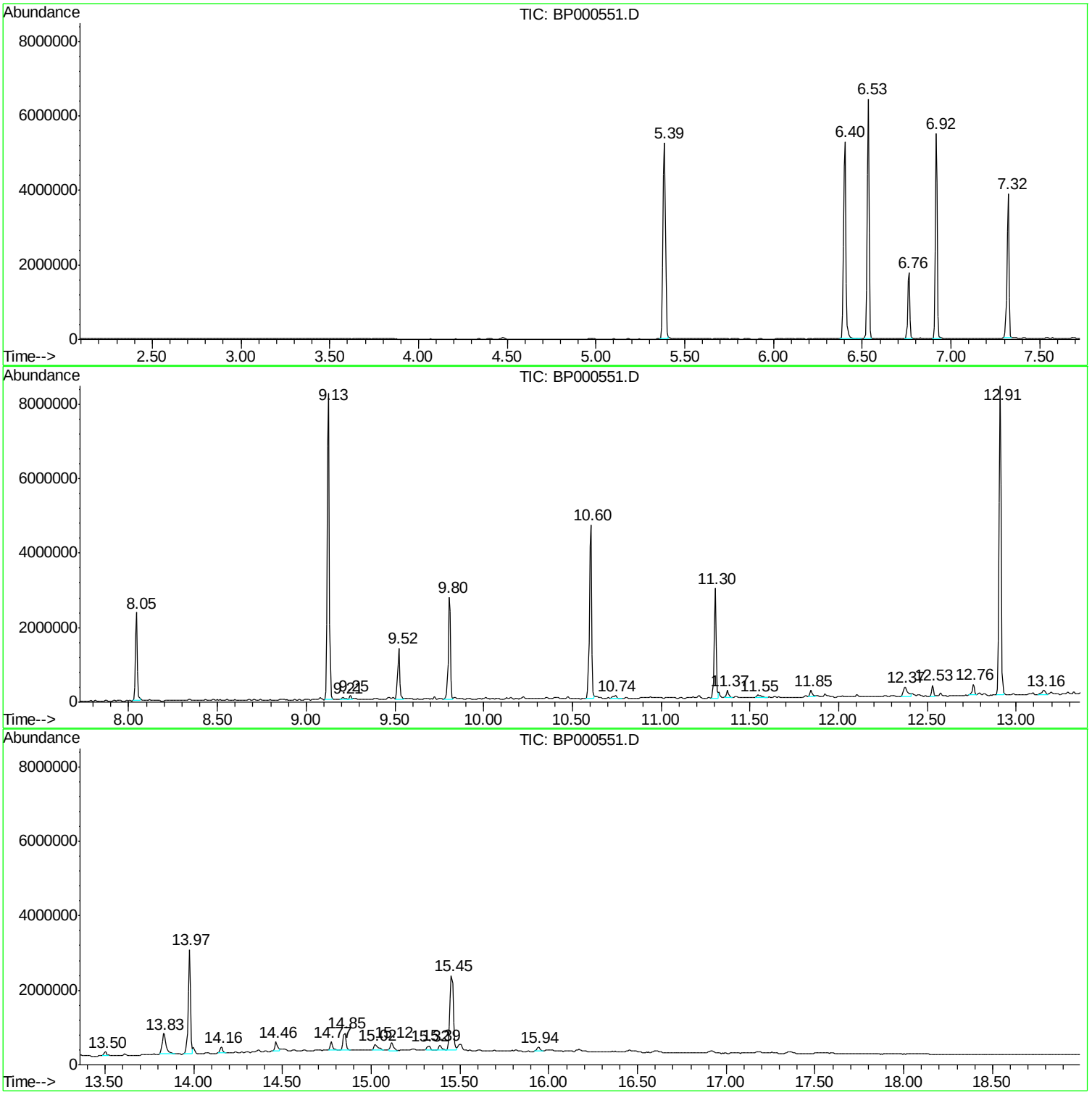
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
Data File : BP000551.D
Acq On : 07 Oct 2019 18:32
Operator : JU
Sample : K5213-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
Data File : BP000551.D
Acq On : 07 Oct 2019 18:32
Operator : JU
Sample : K5213-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

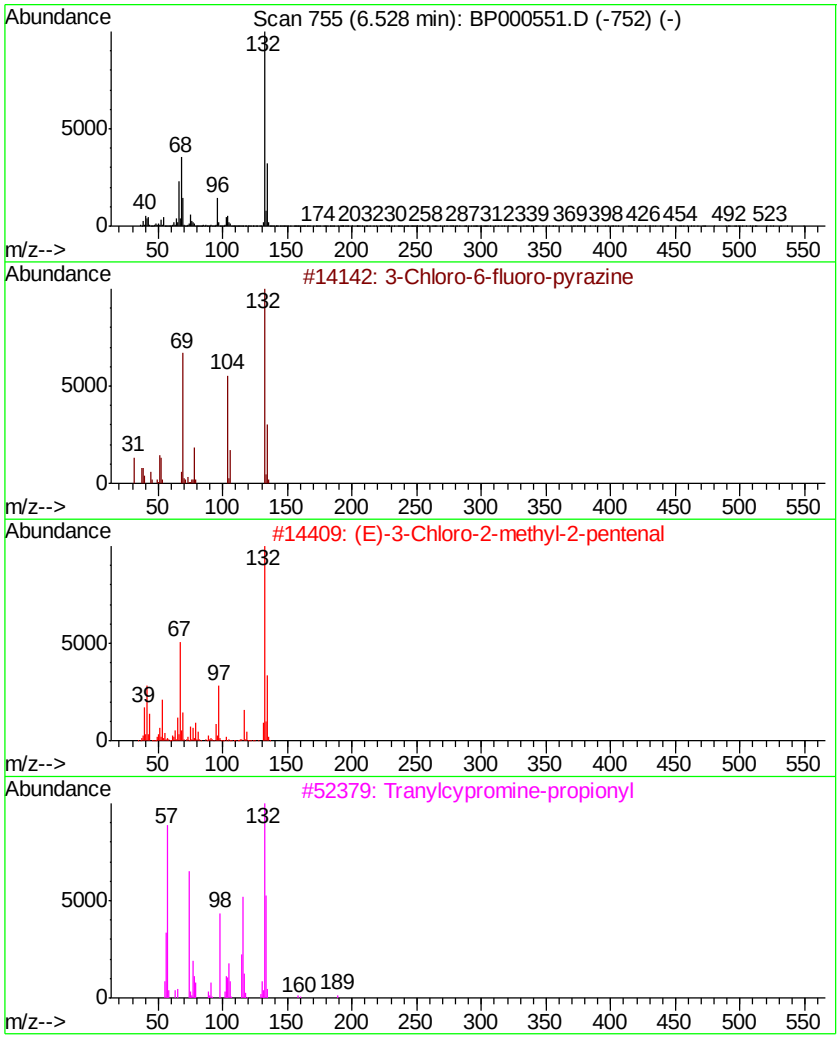
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

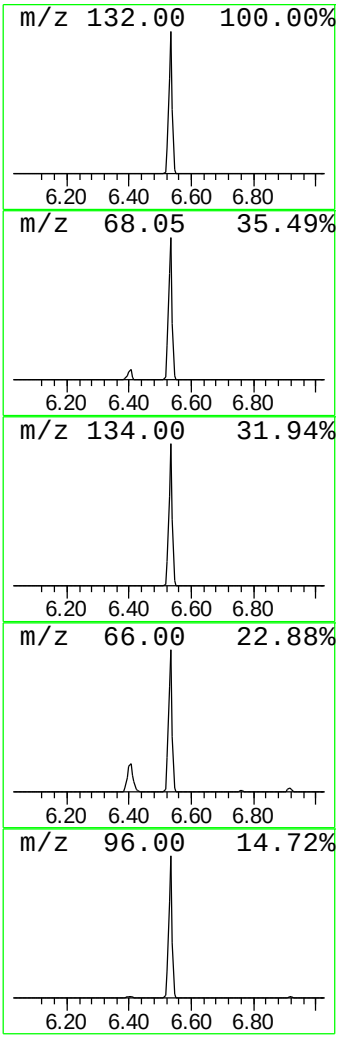
****

Peak Number 1 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	71.56 ng	5415280	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	12





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Operator : JU
Sample : K5213-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

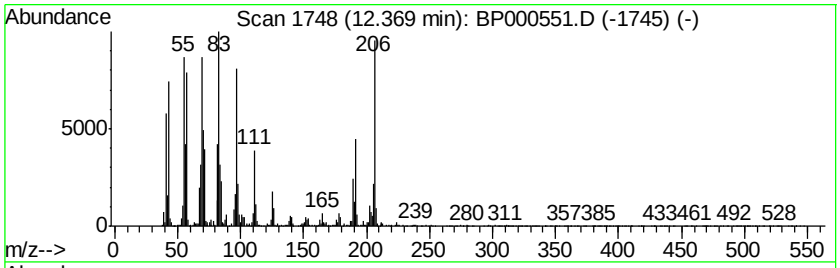
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

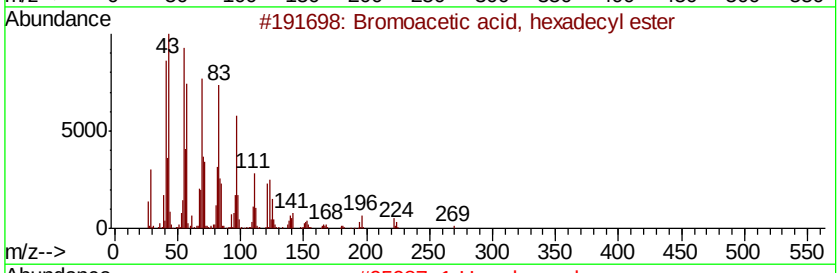
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

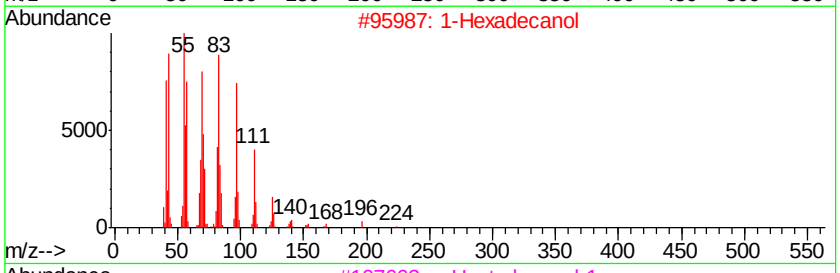
****
Peak Number 3 Bromoacetic acid, hexadecyl... Concentration Rank 5

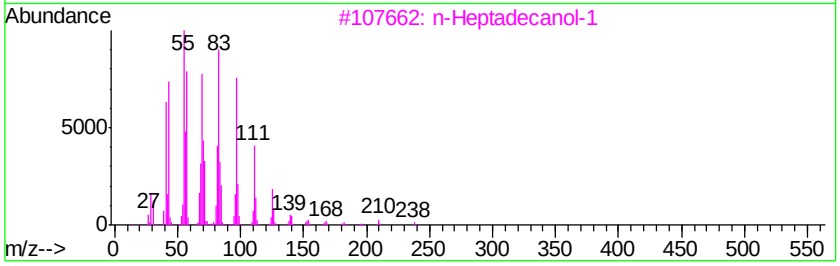
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	3.28 ng	407330	Phenanthrene-d10	11.30

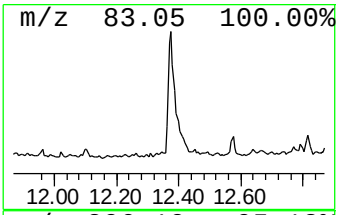
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	83
2	1-Hexadecanol	242	C16H34O	036653-82-4	83
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	83
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	83
5	1-Octadecanol	270	C18H38O	000112-92-5	70

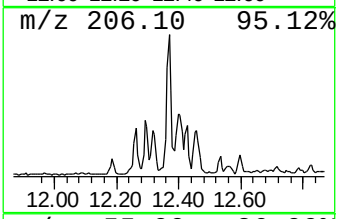


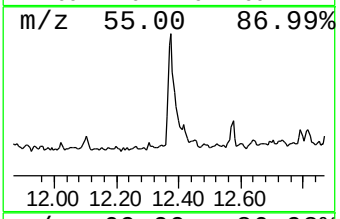


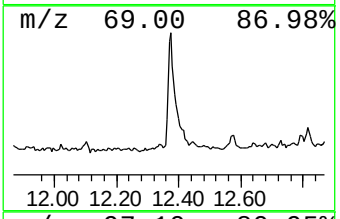


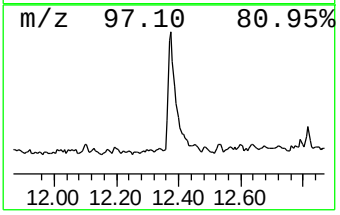












Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP100719\
Data File : BP000551.D
Acq On : 07 Oct 2019 18:32
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Sample : K5213-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

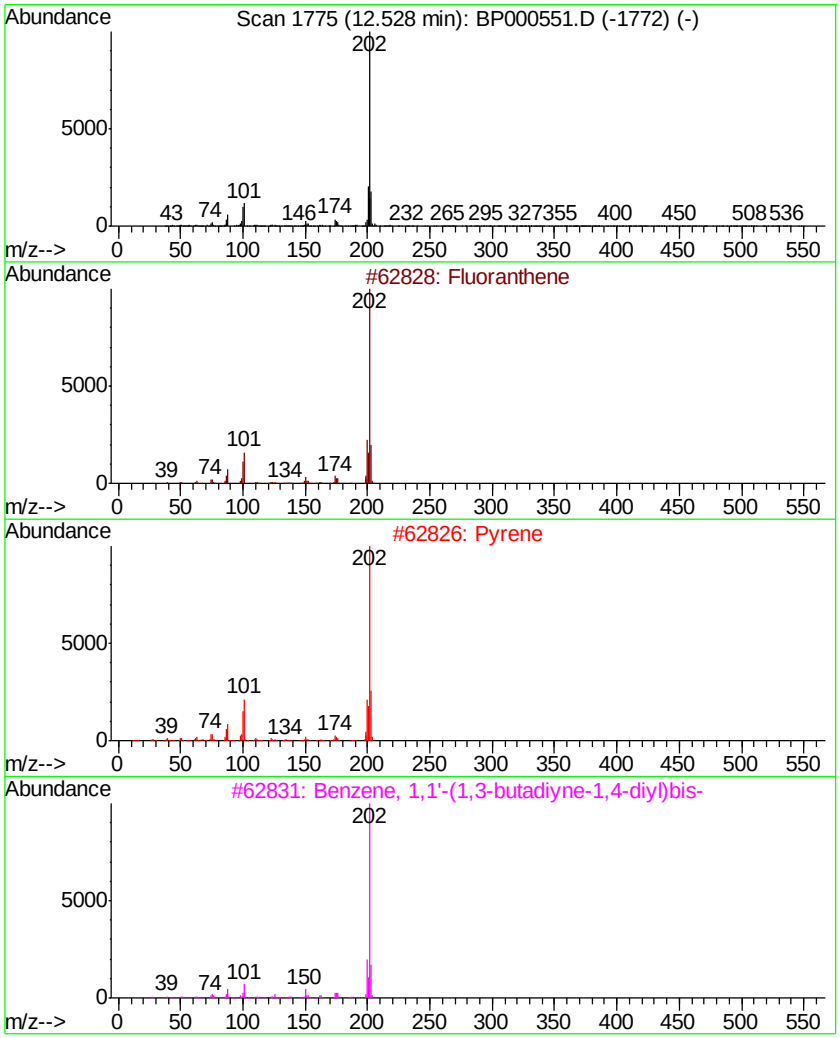
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

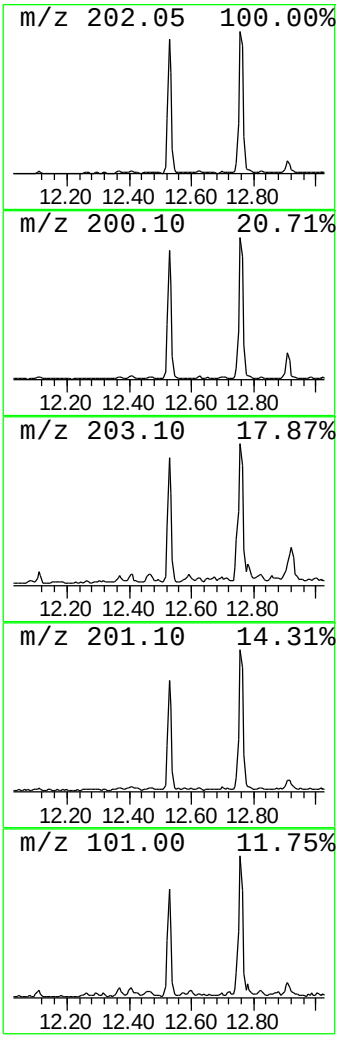
****

Peak Number 4 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	2.09 ng	259912	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	98
2	Pyrene	202	C16H10	000129-00-0	93
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
4	Furan-2-one, 2,5-dihydro-5-(4-me...	202	C12H10O3	024962-84-3	37
5	Succinic acid, di(4-cyanophenyl)...	320	C18H12N2O4	1000360-71-2	28





Library Search Compound Report

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Data File : BP000551.D
Acq On : 07 Oct 2019 18:32
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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
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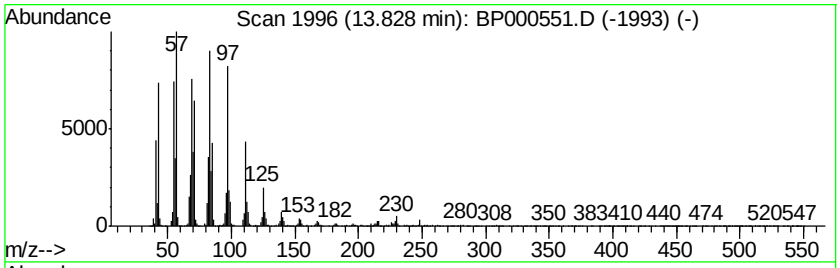
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

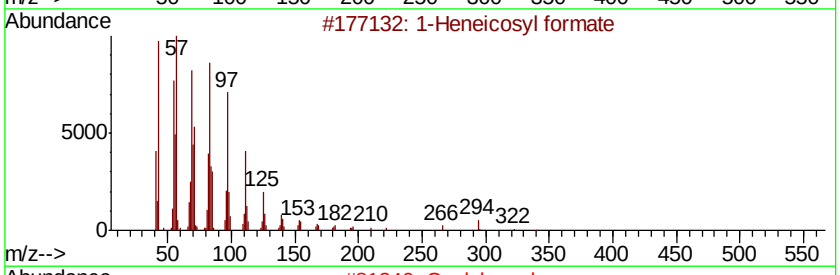
****

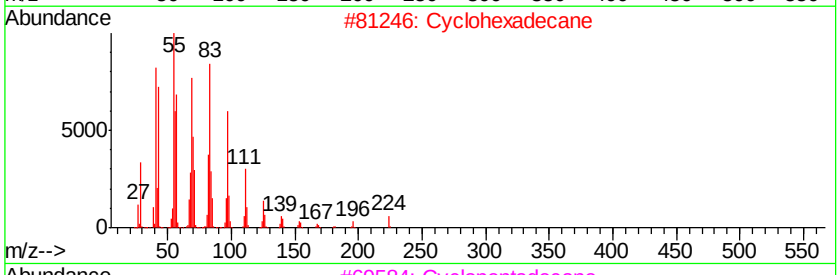
Peak Number 5 1-Heneicosyl formate Concentration Rank 3

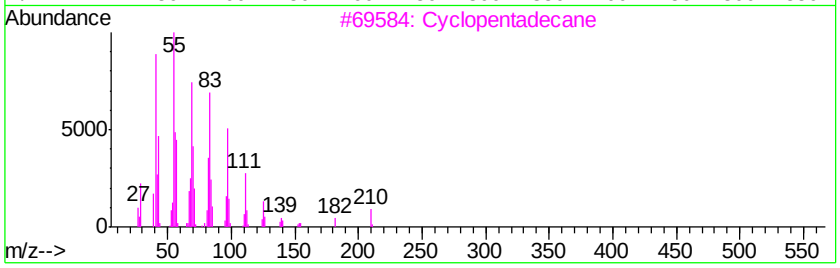
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	6.10 ng	799092	Chrysene-d12	13.97

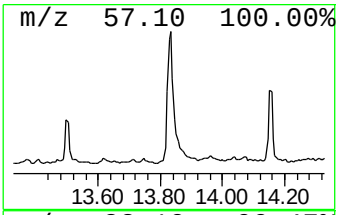
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	99
2	Cyclohexadecane	224	C16H32	000295-65-8	94
3	Cyclopentadecane	210	C15H30	000295-48-7	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	94

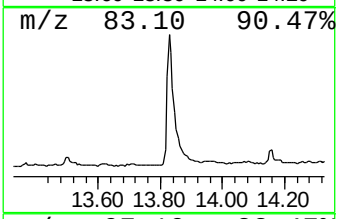


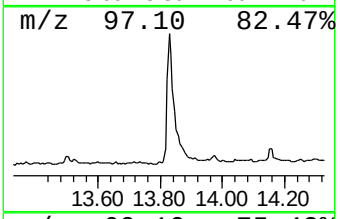


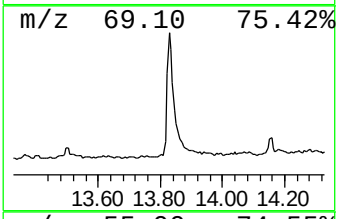


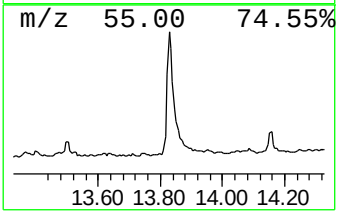












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Instrument : BNA_P
ClientSampleId : S-4(5-10)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

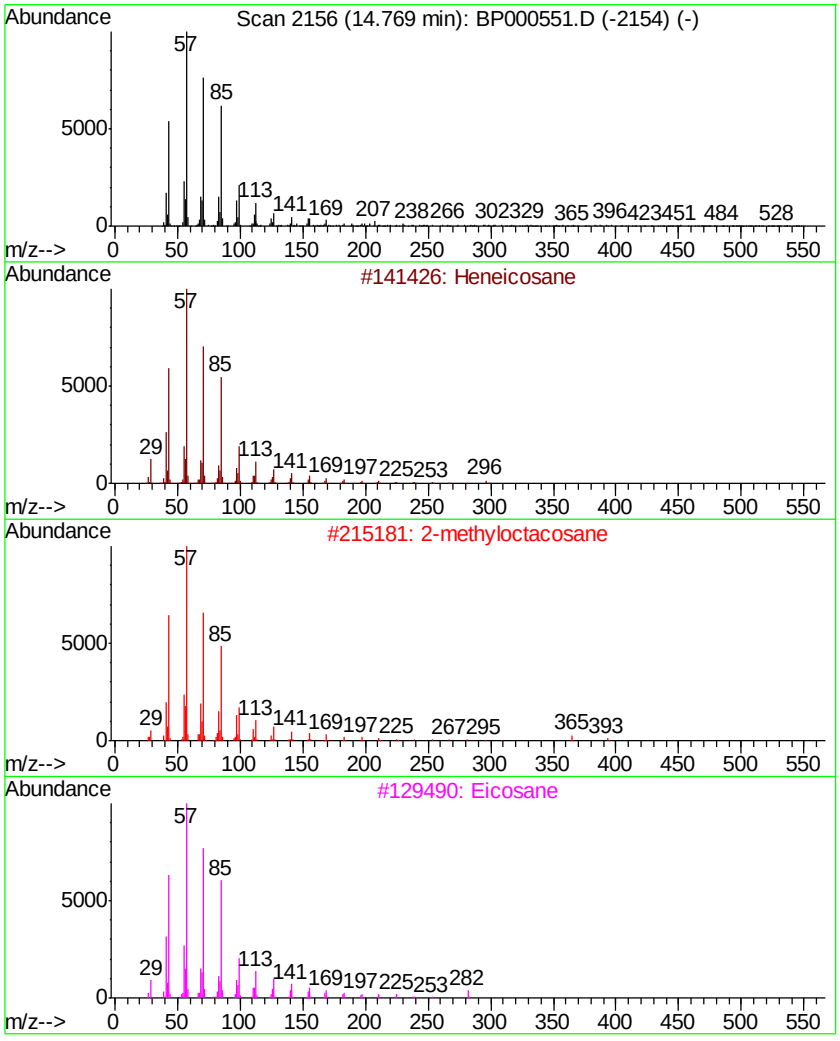
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

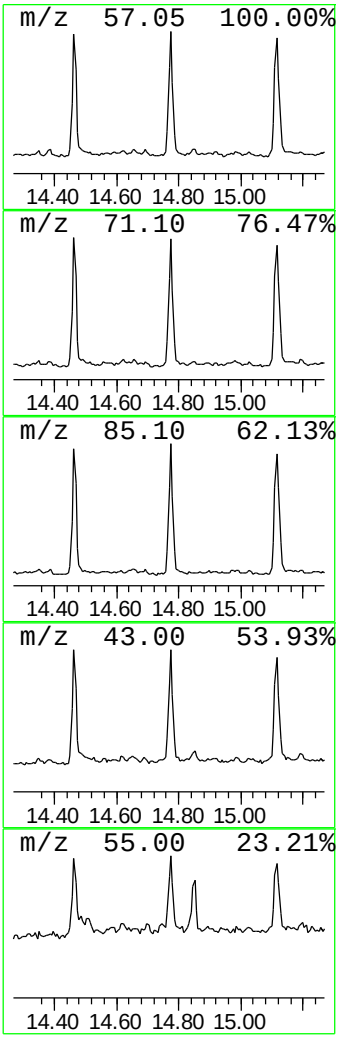
****

Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	2.11 ng	258760	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octacosane	394	C28H58	000630-02-4	87





Library Search Compound Report

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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

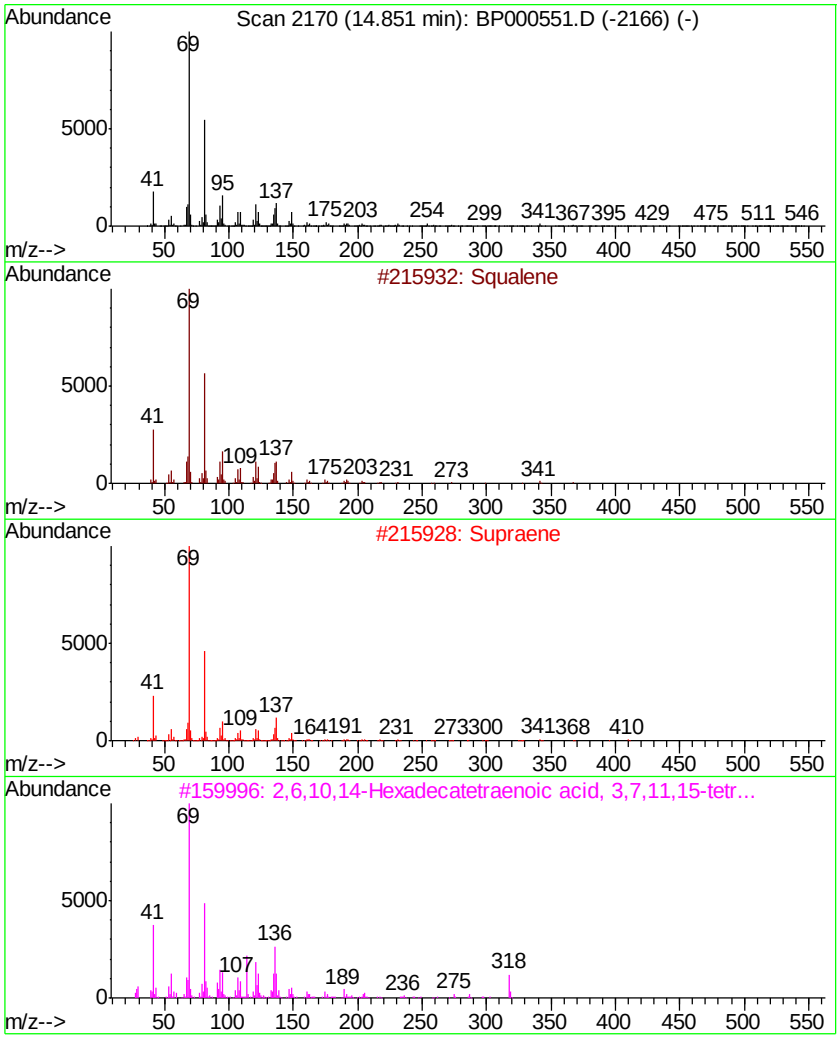
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

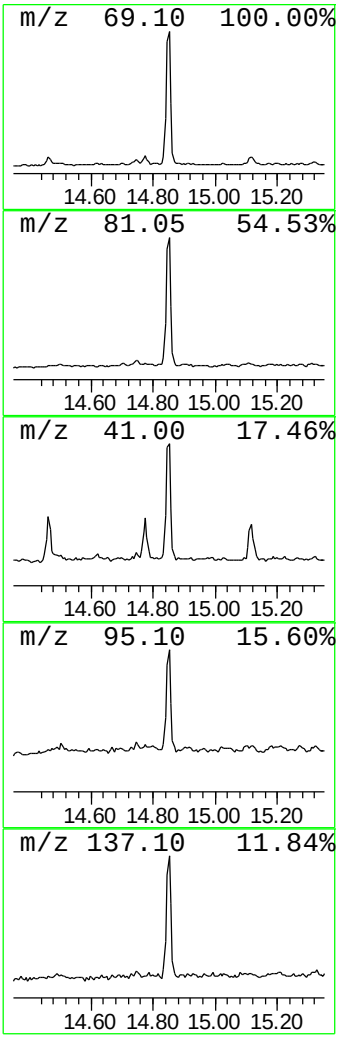
****

Peak Number 7 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	3.87 ng	473680	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	95
2	Supraene	410	C30H50	007683-64-9	91
3	2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	78
4	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59
5	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52





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Data File : BP000551.D
Acq On : 07 Oct 2019 18:32
Operator : JU
Sample : K5213-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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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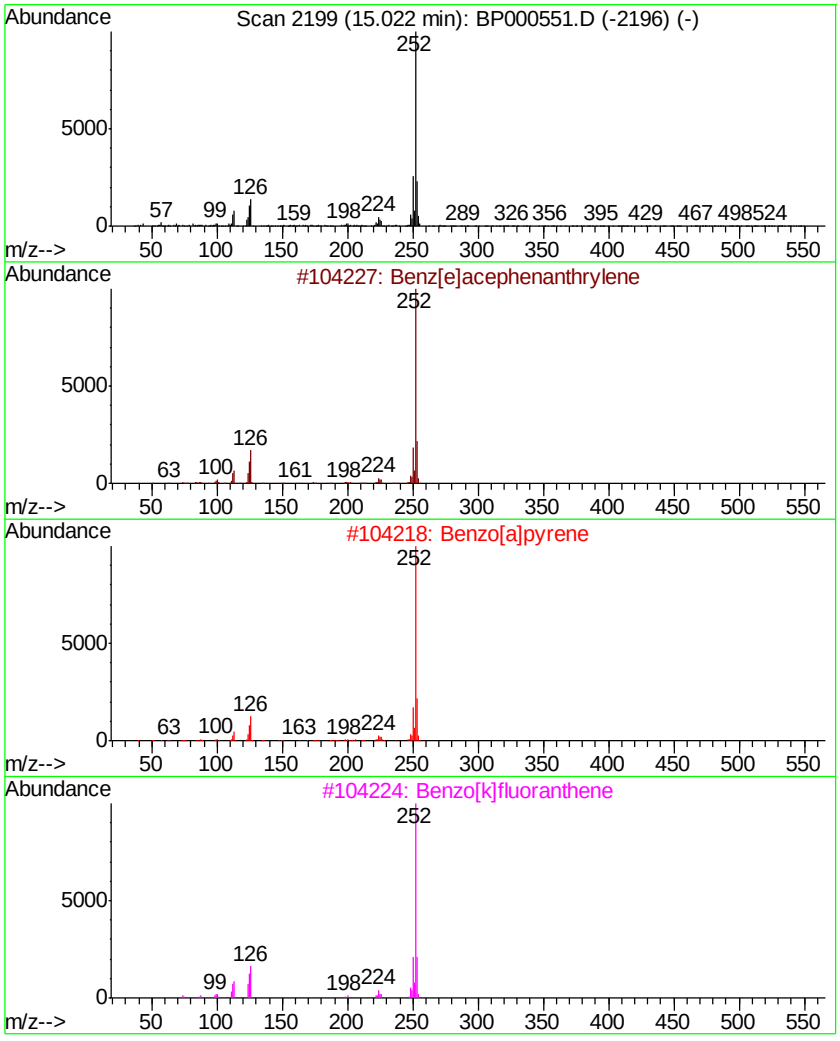
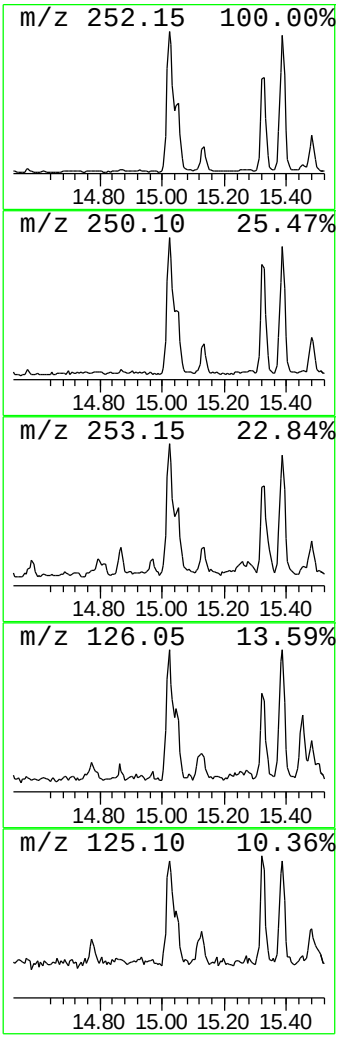
Peak Number 8 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.29 ng	280550	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	94
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4	Benzo[e]pyrene	252	C20H12	000192-97-2	91
5	Perylene	252	C20H12	000198-55-0	87





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Data File : BP000551.D
Acq On : 07 Oct 2019 18:32
Operator : JU
Sample : K5213-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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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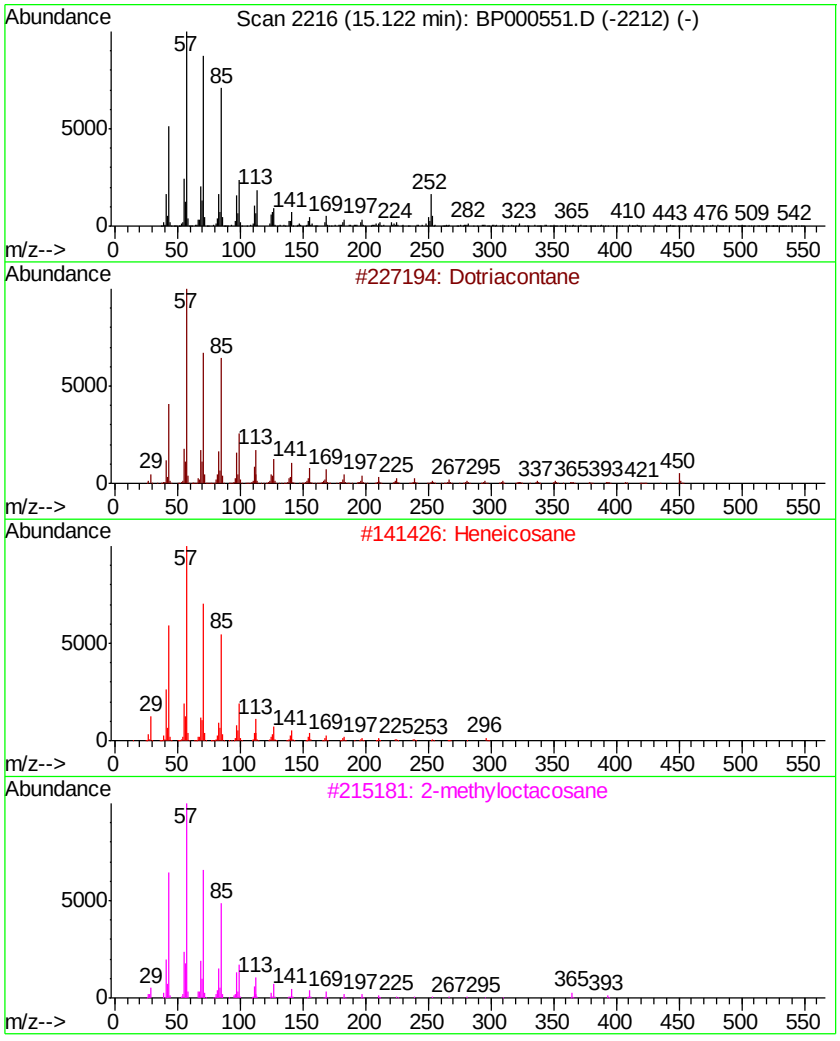
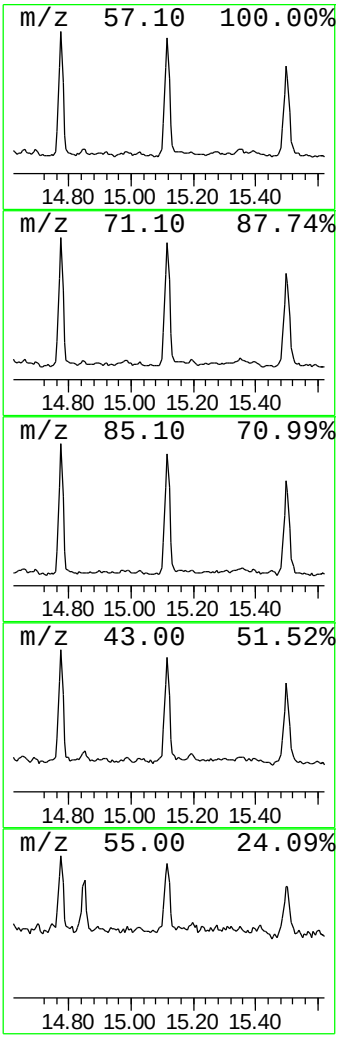
Peak Number 9 Dotriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	2.21 ng	271233	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontane	451	C32H66	000544-85-4	96
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Triacontane	422	C30H62	000638-68-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP100719\
Data File : BP000551.D
Acq On : 07 Oct 2019 18:32
Operator : JU
Sample : K5213-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-4(5-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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
unknown6.53	6.53	71.6	ng	5415280	1	6.76	1513470	20.0
Bromoacetic acid,...	12.37	3.3	ng	407330	4	11.30	2485670	20.0
Benzene, 1,1'-(1,...	12.53	2.1	ng	259912	4	11.30	2485670	20.0
1-Heneicosyl formate	13.83	6.1	ng	799092	5	13.97	2619090	20.0
Heneicosane	14.77	2.1	ng	258760	6	15.45	2450760	20.0
Squalene	14.85	3.9	ng	473680	6	15.45	2450760	20.0
Benzo[e]pyrene	15.02	2.3	ng	280550	6	15.45	2450760	20.0
Dotriacontane	15.12	2.2	ng	271233	6	15.45	2450760	20.0