LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081920\
Data File : BP003042.D
Acq On : 19 Aug 2020 20:37
Operator : CG/JU
Sample : L3712-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

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-BP073020.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	2.952	7	11	27	rVB	1361748	1598053	23.19%	2.356%
2	4.822	324	329	340	rVB2	72428	105968	1.54%	0.156%
3	5.287	400	408	428	rBV	2821768	4165066	60.45%	6.142%
4	6.393	590	596	603	rVB	87666	131384	1.91%	0.194%
5	6.858	666	675	690	rBV	2604503	4262952	61.87%	6.286%
6	7.681	807	815	825	rBV	1146873	1777623	25.80%	2.621%
7	7.916	845	855	861	rBV	129687	204558	2.97%	0.302%
8	8.822	998	1009	1024	rBV	1742798	2881521	41.82%	4.249%
9	10.457	1279	1287	1299	rBV	1573145	2712341	39.36%	4.000%
10	11.169	1403	1408	1414	rVB6	70558	147180	2.14%	0.217%
11	11.522	1463	1468	1471	rBV3	82283	157340	2.28%	0.232%
12	11.946	1533	1540	1547	rBV10	82280	293420	4.26%	0.433%
13	12.216	1582	1586	1593	rBV5	115043	242142	3.51%	0.357%
14	12.481	1627	1631	1636	rBV5	61720	140069	2.03%	0.207%
15	12.887	1696	1700	1702	rBV2	139033	181990	2.64%	0.268%
16	12.940	1703	1709	1718	rVV	4638970	6890357	100.00%	10.161%
17	13.116	1731	1739	1742	rBV3	337301	753372	10.93%	1.111%
18	13.263	1761	1764	1769	rVB4	191073	264817	3.84%	0.391%
19	13.604	1818	1822	1825	rBV4	328677	488974	7.10%	0.721%
20	13.681	1832	1835	1842	rVB	966385	1469230	21.32%	2.167%
21	13.751	1843	1847	1856	rBV3	978969	2317331	33.63%	3.417%
22	14.163	1914	1917	1926	rVB	1314478	2168791	31.48%	3.198%
23	14.240	1927	1930	1935	rBV4	403139	640005	9.29%	0.944%
24	14.316	1936	1943	1948	rBV2	2465949	5236709	76.00%	7.722%
25	14.663	1999	2002	2005	rBV	562748	792983	11.51%	1.169%
26	15.128	2077	2081	2087	rVB2	1691647	2576848	37.40%	3.800%
27	15.816	2195	2198	2207	rVB2	1870081	2670134	38.75%	3.937%
28	19.651	2847	2850	2855	rVB	4935640	6424796	93.24%	9.474%
29	20.898	3059	3062	3067	rVV2	1111572	1525002	22.13%	2.249%
30	20.951	3068	3071	3079	rVB	869929	1208972	17.55%	1.783%
31	21.163	3103	3107	3112	rVB	3043617	3912278	56.78%	5.769%
32	21.816	3215	3218	3224	rVB	765144	1006988	14.61%	1.485%
33	22.233	3286	3289	3301	rVB2	500337	810758	11.77%	1.196%
34	22.757	3369	3378	3383	rBV2	945628	1952230	28.33%	2.879%

LSC Area Percent Report

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Misc :
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Instrument : BNA_P
ClientSampleId : CHRT-25433

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-BP073020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.404	3482	3488	3503	rVB2	2510915	4926156	71.49%	7.264%
36	23.998	3585	3589	3596	rVB	407160	776396	11.27%	1.145%

Sum of corrected areas: 67814734

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081920\
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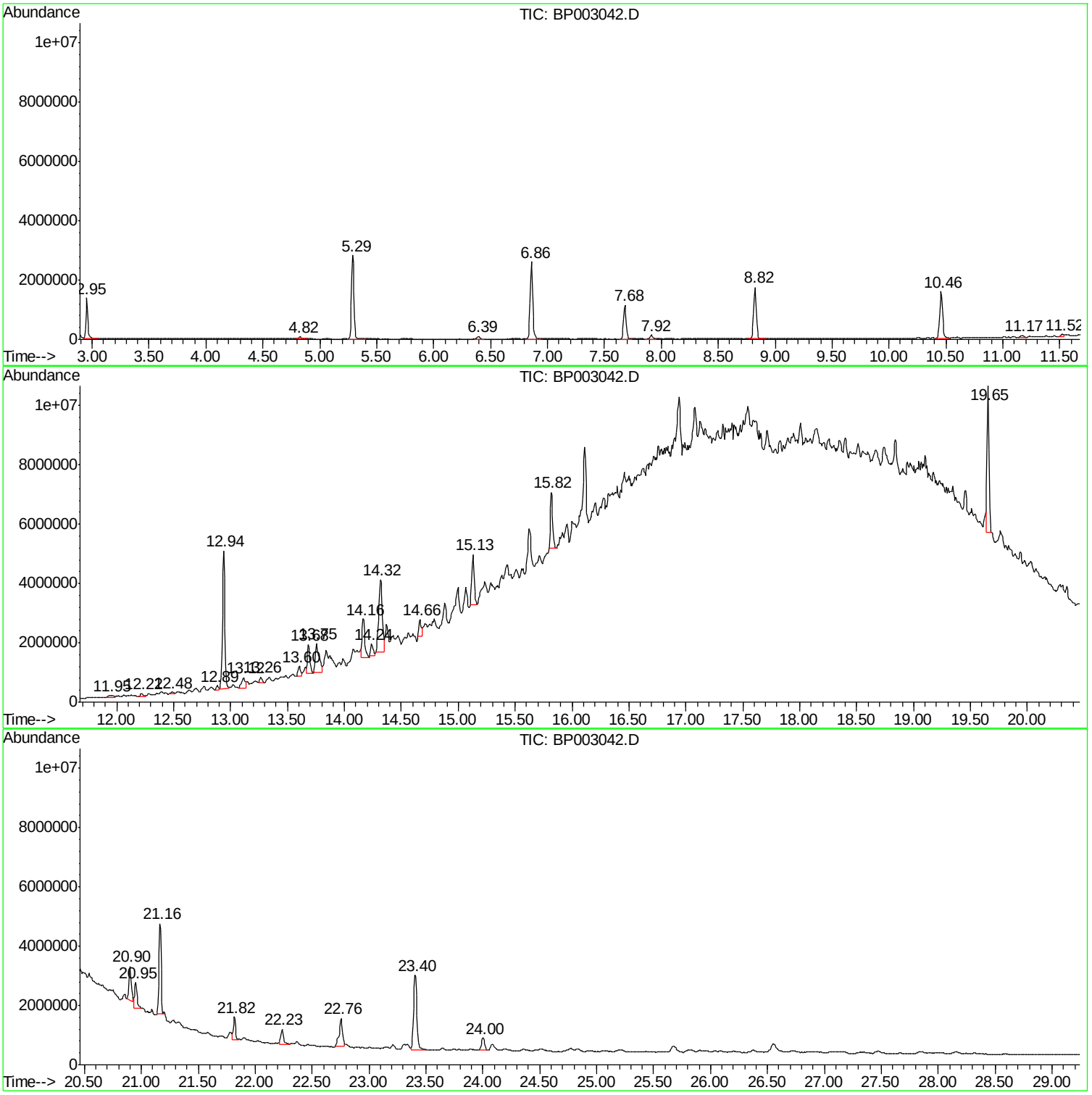
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.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 P\DATA\BP081920\
Data File : BP003042.D
Acq On : 19 Aug 2020 20:37
Operator : CG/JU
Sample : L3712-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

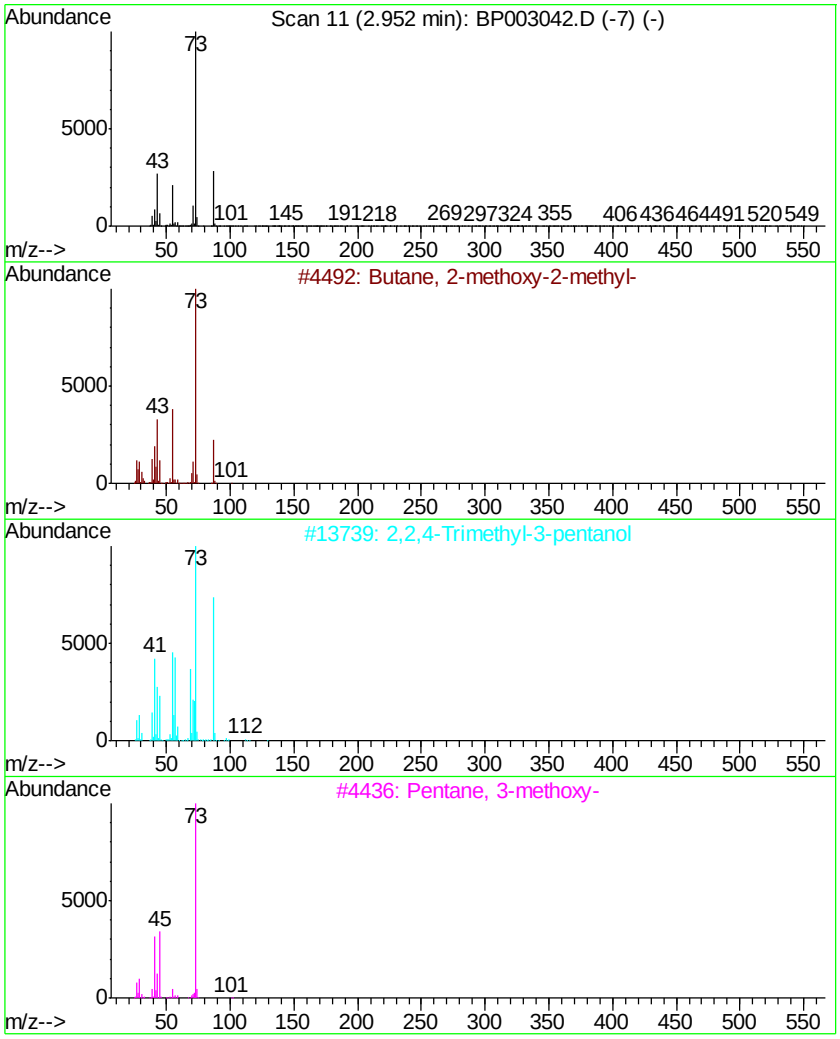
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

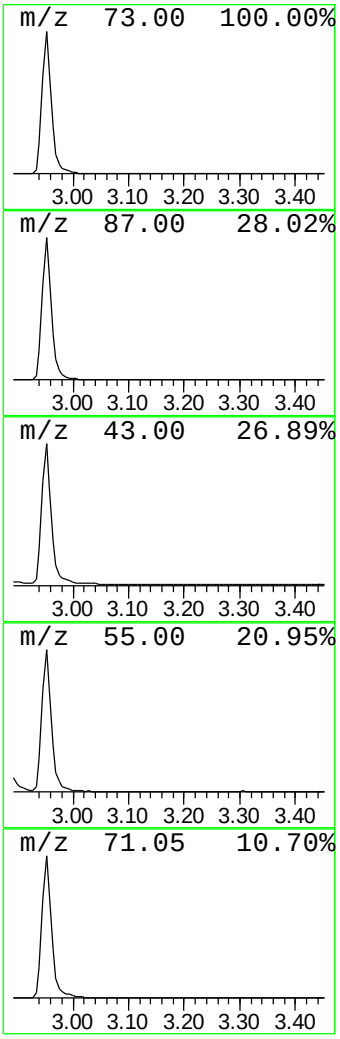
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.95	17.98 ng	1598050	1,4-Dichlorobenzene-d4	7.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081920\
Data File : BP003042.D
Acq On : 19 Aug 2020 20:37
Operator : CG/JU
Sample : L3712-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

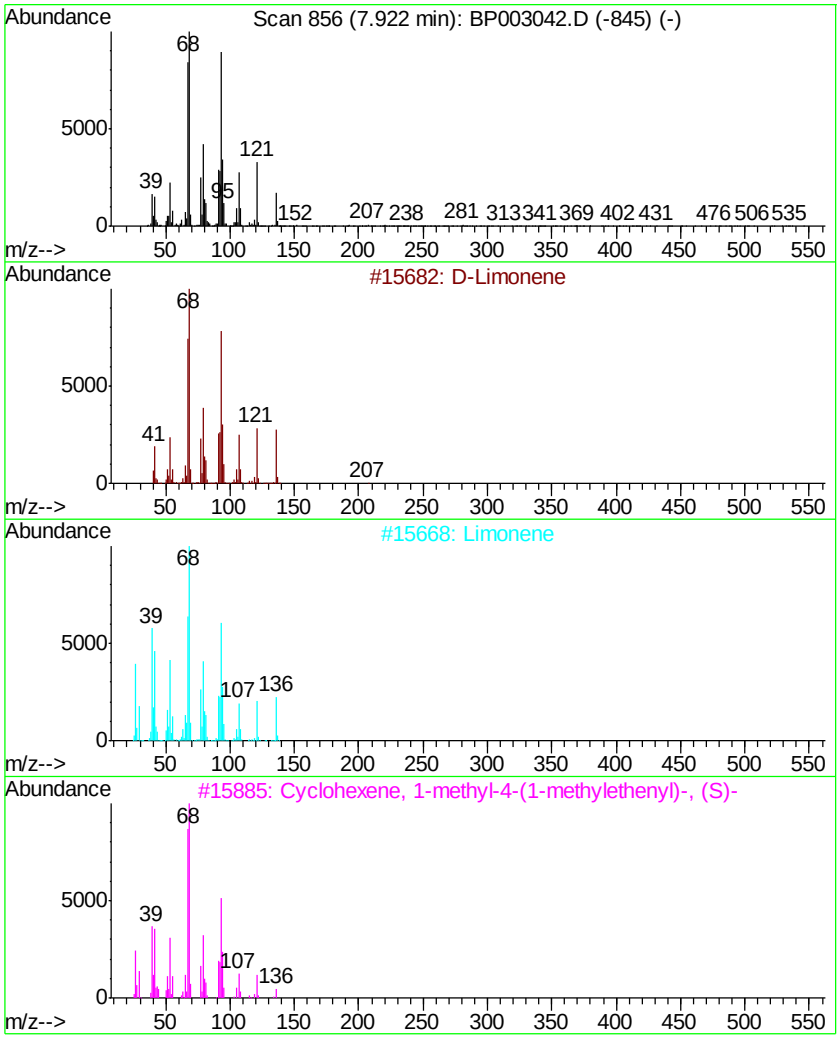
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

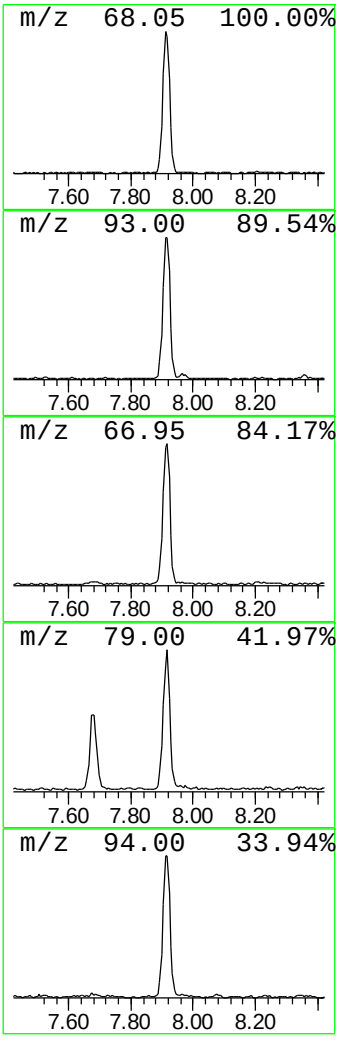
****

Peak Number 2 D-Limonene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.92	2.30 ng	204558	1,4-Dichlorobenzene-d4	7.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	98
2	Limonene	136	C10H16	000138-86-3	91
3	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	90
4	Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	70
5	Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081920\
Data File : BP003042.D
Acq On : 19 Aug 2020 20:37
Operator : CG/JU
Sample : L3712-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

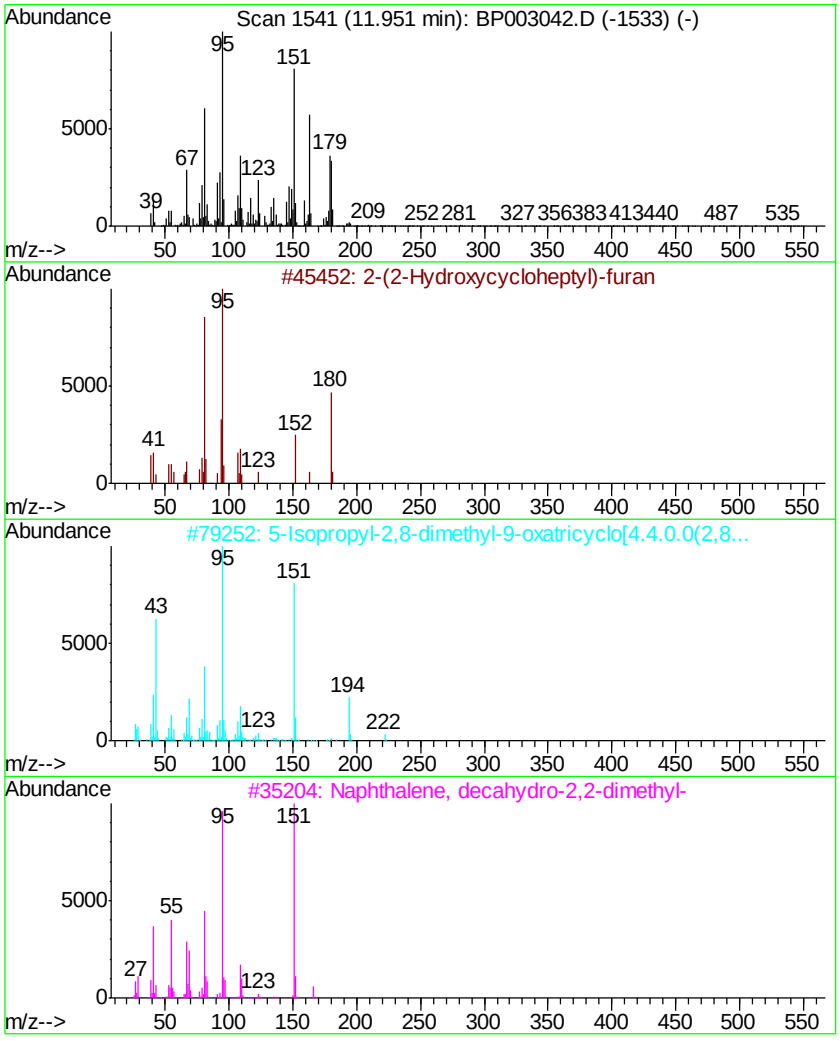
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

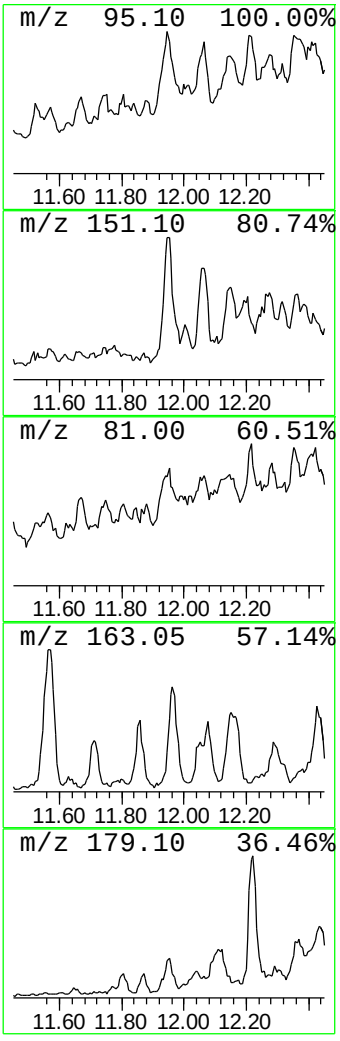
****

Peak Number 3 unknown11.95 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.16 ng	293420	Naphthalene-d8	10.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Hydroxycycloheptyl)-furan	180	C11H16O2	1000145-02-9	45
2	5-Isopropyl-2,8-dimethyl-9-oxatr...	222	C14H22O2	1000185-23-8	38
3	Naphthalene, decahydro-2,2-dimet...	166	C12H22	031124-85-3	38
4	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	38
5	Bicyclo[3.3.1]nonan-9-one, 1,2,4...	225	C12H19NO3	129967-65-3	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081920\
Data File : BP003042.D
Acq On : 19 Aug 2020 20:37
Operator : CG/JU
Sample : L3712-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

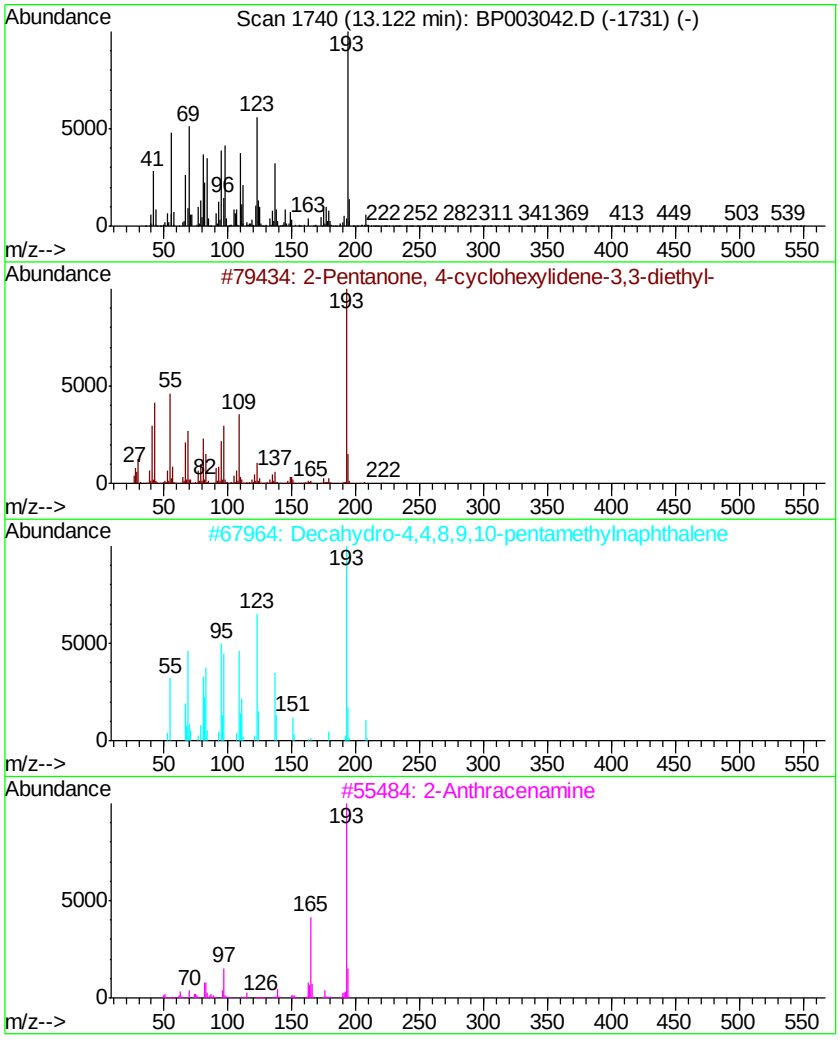
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

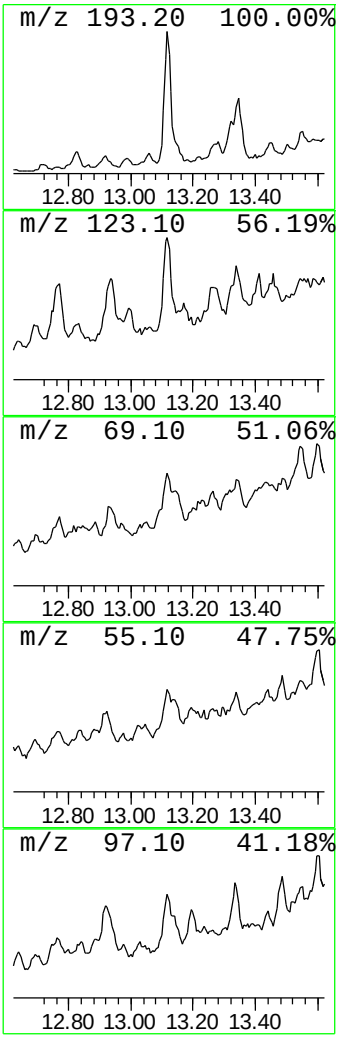
****

Peak Number 4 2-Pentanone, 4-cyclohexylid... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	2.88 ng	753372	Acenaphthene-d10	14.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	70
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	64
3	2-Anthracenamine	193	C14H11N	000613-13-8	35
4	9-Phenanthrenamine	193	C14H11N	000947-73-9	25
5	s-Triazine, 2-amino-4-piperidino...	262	C13H22N6	022404-26-8	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081920\
Data File : BP003042.D
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Sample : L3712-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.M
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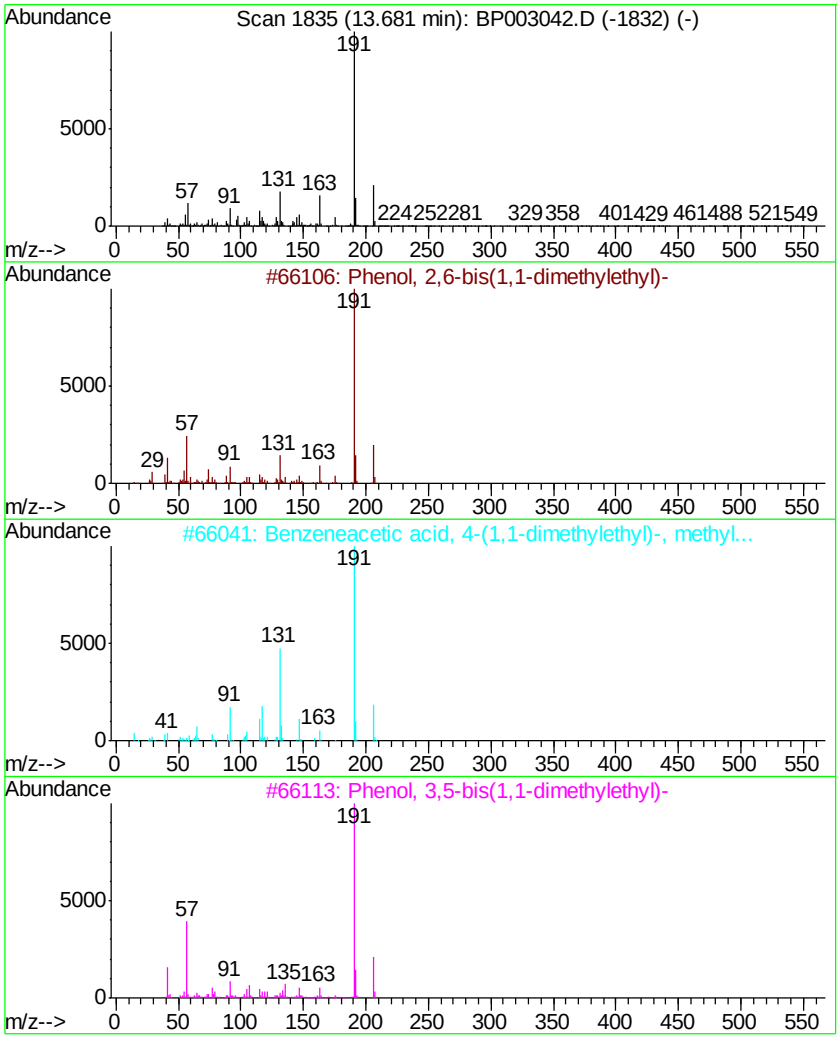
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

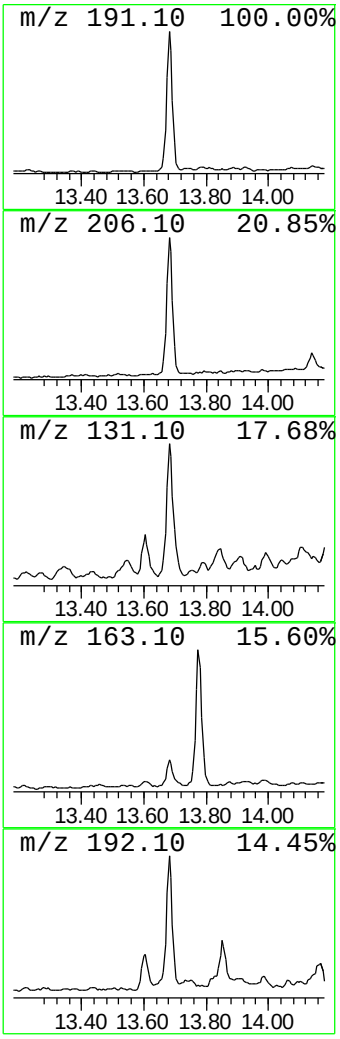
****

Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	5.61 ng	1469230	Acenaphthene-d10	14.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	94
2	Benzeneacetic acid, 4-(1,1-dimet...	206	C13H18O2	003549-23-3	80
3	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	74
4	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	72
5	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	72





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Instrument : BNA_P
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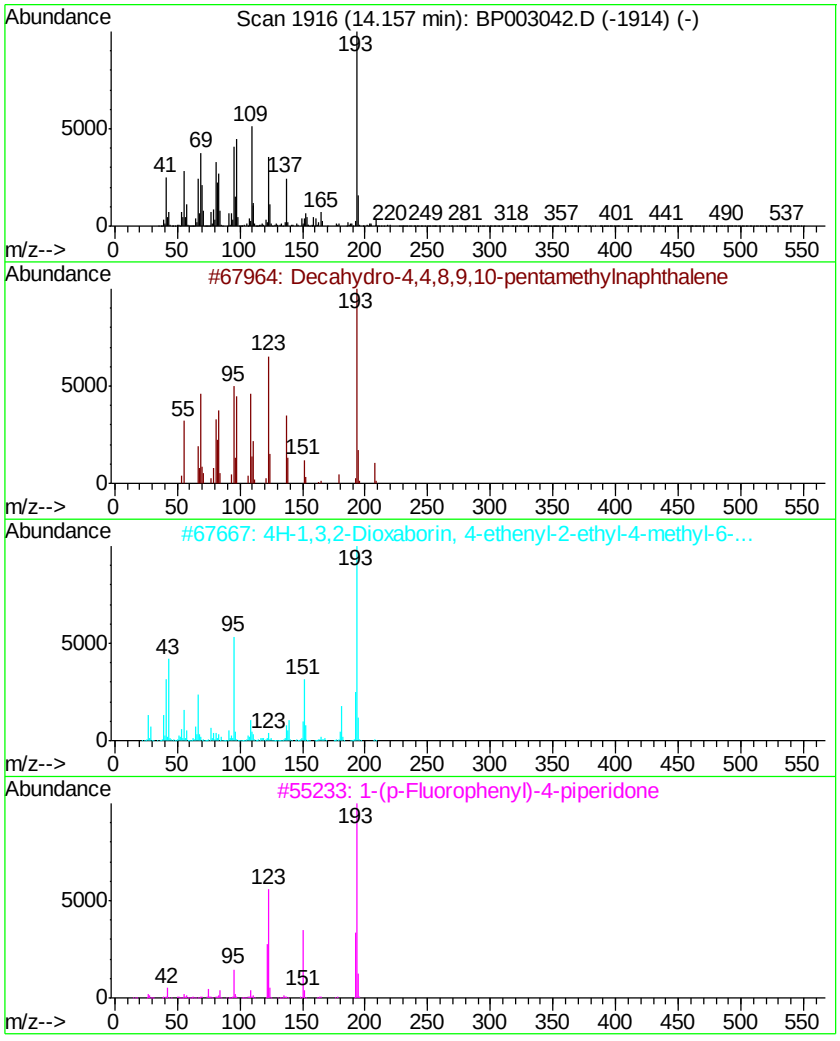
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

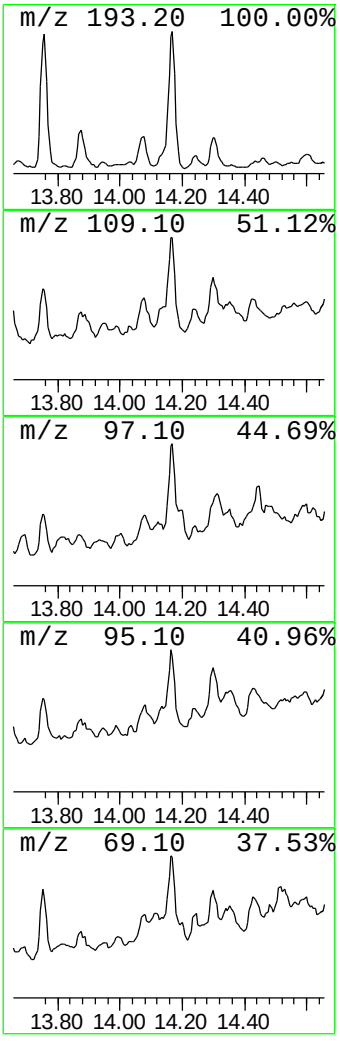
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Decahydro-4,4,8,9,10-pentam... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	8.28 ng	2168790	Acenaphthene-d10	14.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	60
2	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21BO2	074630-04-9	38
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
4	Boronic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	25
5	6-Methylphenanthridine	193	C14H11N	003955-65-5	22





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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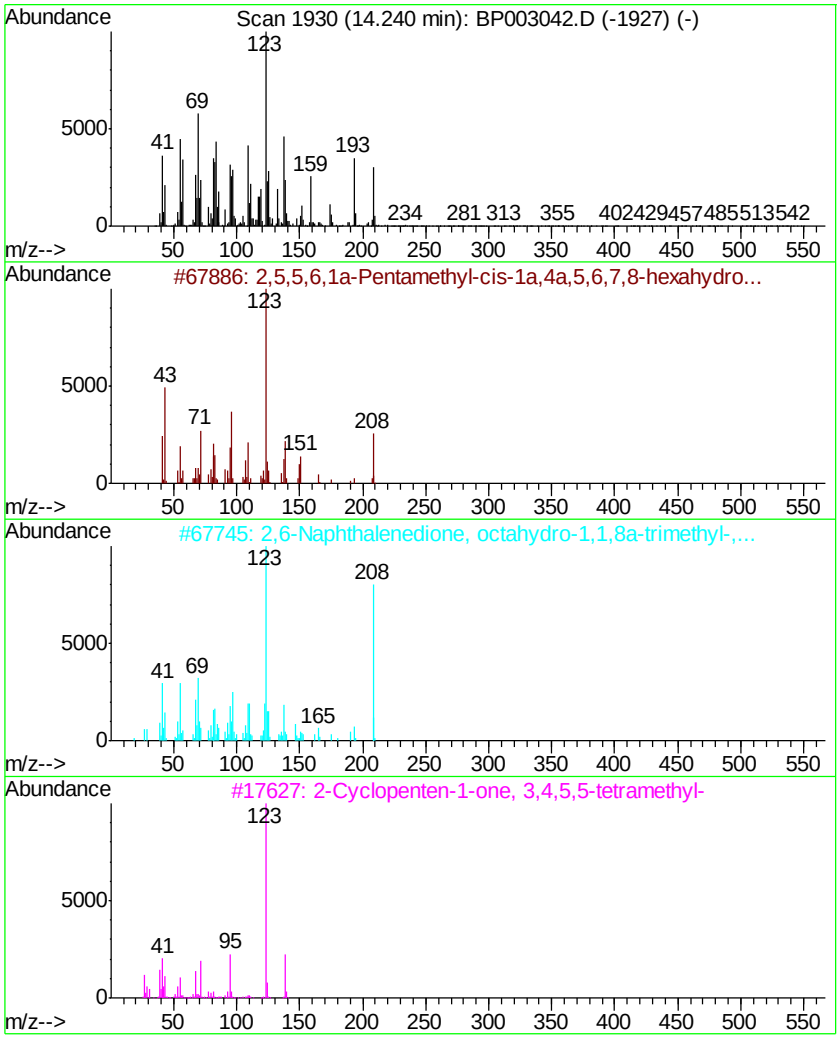
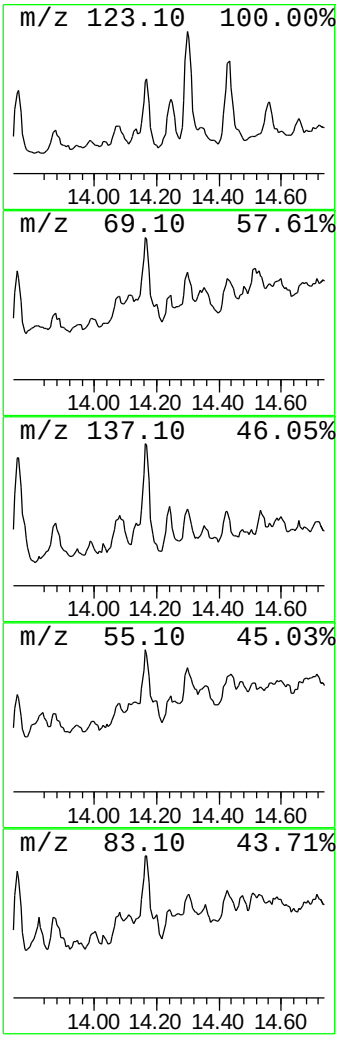
****

Peak Number 7 unknown14.24 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	2.44 ng	640005	Acenaphthene-d10	14.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,5,6,1a-Pentamethyl-cis-1a,4a...	208	C14H24O	1000215-77-9	37
2	2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	32
3	2-Cyclopenten-1-one, 3,4,5,5-tet...	138	C9H14O	090611-02-2	25
4	Cyclohexene, 1,4,6,6-tetramethyl-	138	C10H18	070092-37-4	22
5	1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	22





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Data File : BP003042.D
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Operator : CG/JU
Sample : L3712-11
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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

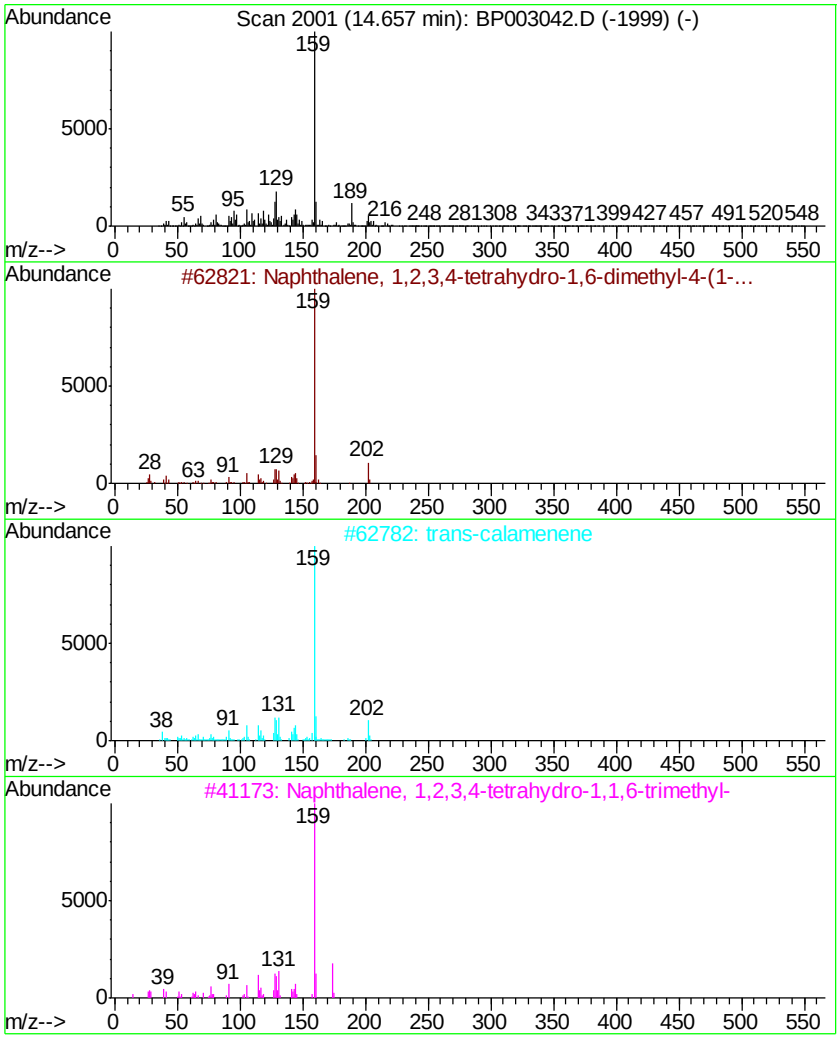
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

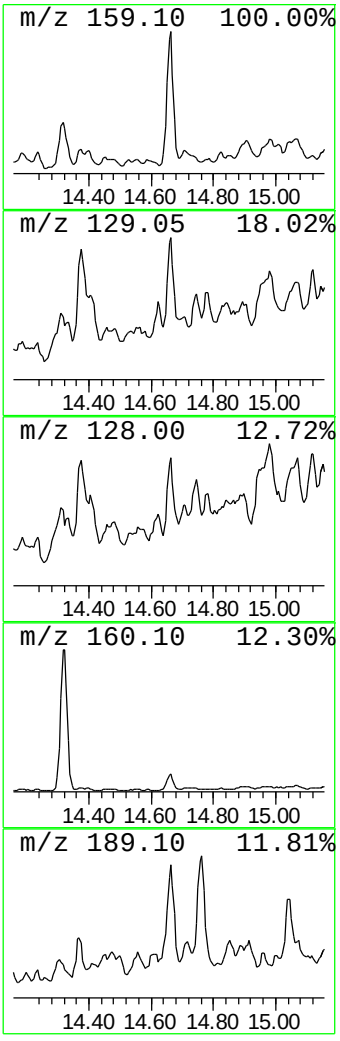
****

Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.03 ng	792983	Acenaphthene-d10	14.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	202	C15H22	000483-77-2	83
2	trans-calamenene	202	C15H22	1000374-17-3	74
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	72
4	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	72
5	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-51-6	64





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Acq On : 19 Aug 2020 20:37
Operator : CG/JU
Sample : L3712-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.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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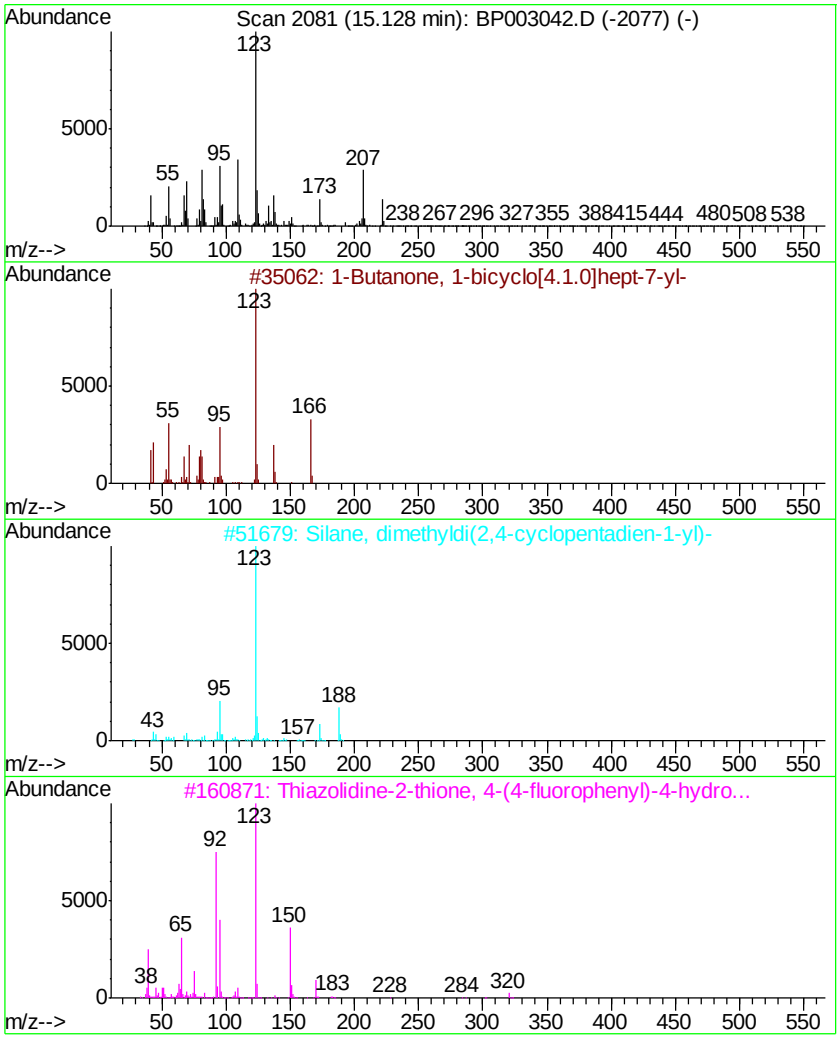
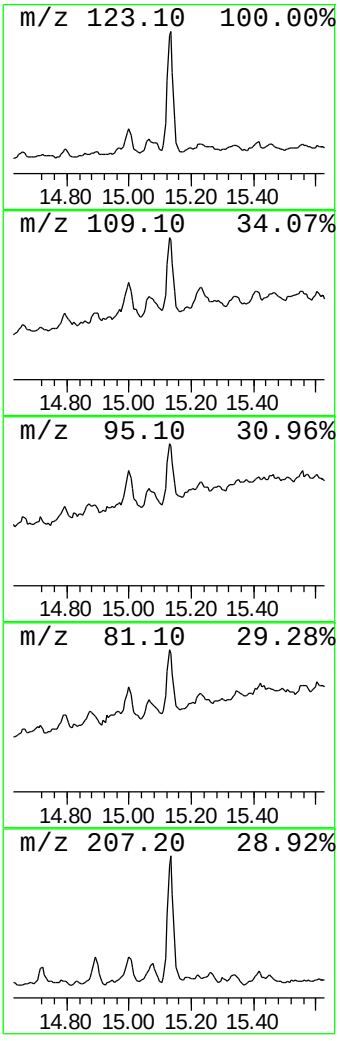
Peak Number 9 unknown15.13 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	9.84 ng	2576850	Acenaphthene-d10	14.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanone, 1-bicyclo[4.1.0]hept...	166	C11H18O	054764-62-4	43
2	Silane, dimethyldi(2,4-cyclopent...	188	C12H16Si	018053-74-2	43
3	Thiazolidine-2-thione, 4-(4-fluo...	320	C15H13FN2OS2	1000264-97-7	43
4	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	38
5	4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	38





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Sample : L3712-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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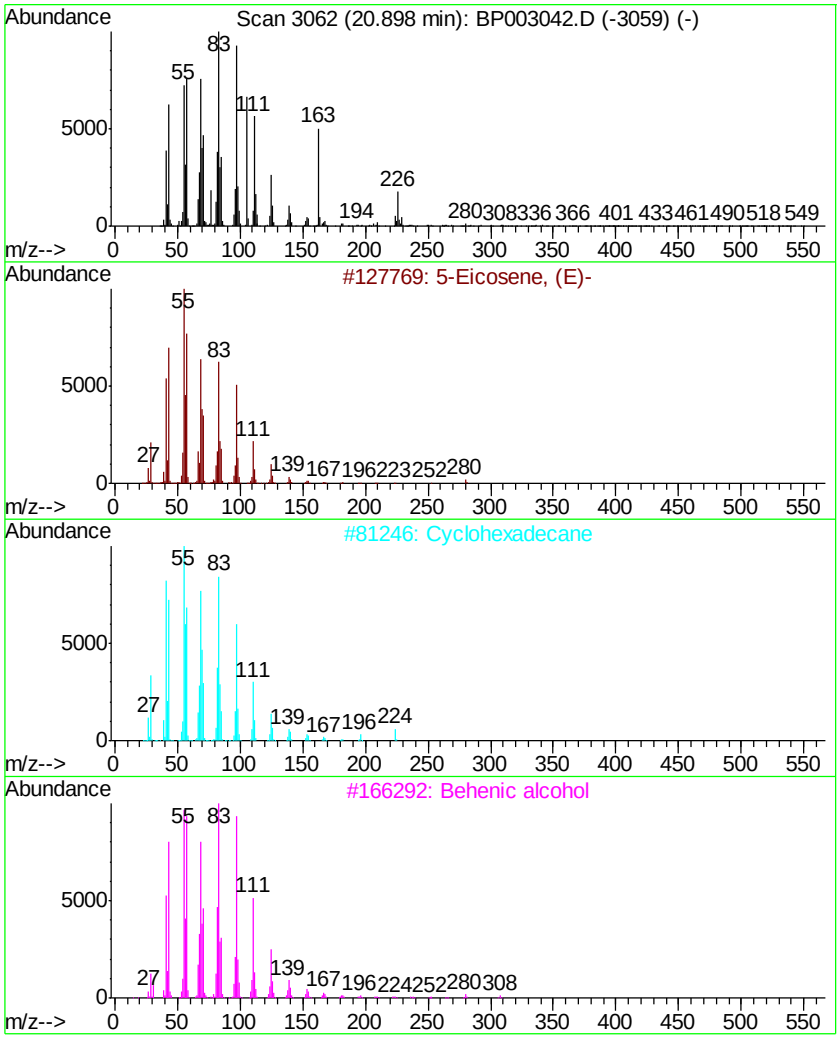
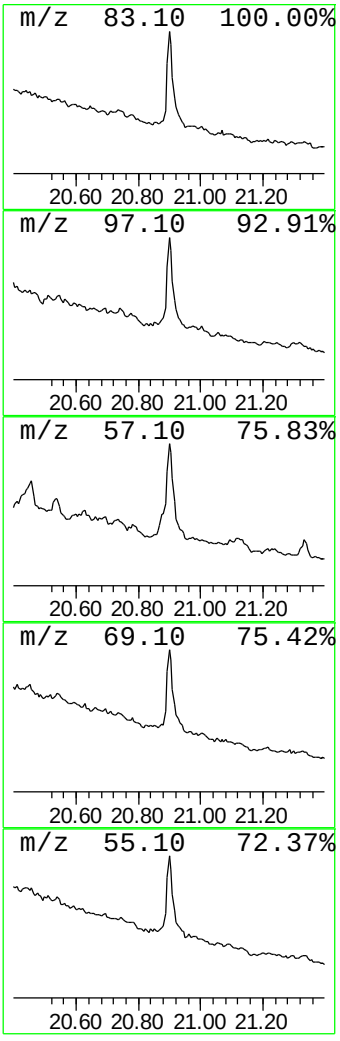
Peak Number 10 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.90	7.80 ng	1525000	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	Cyclohexadecane	224	C16H32	000295-65-8	96
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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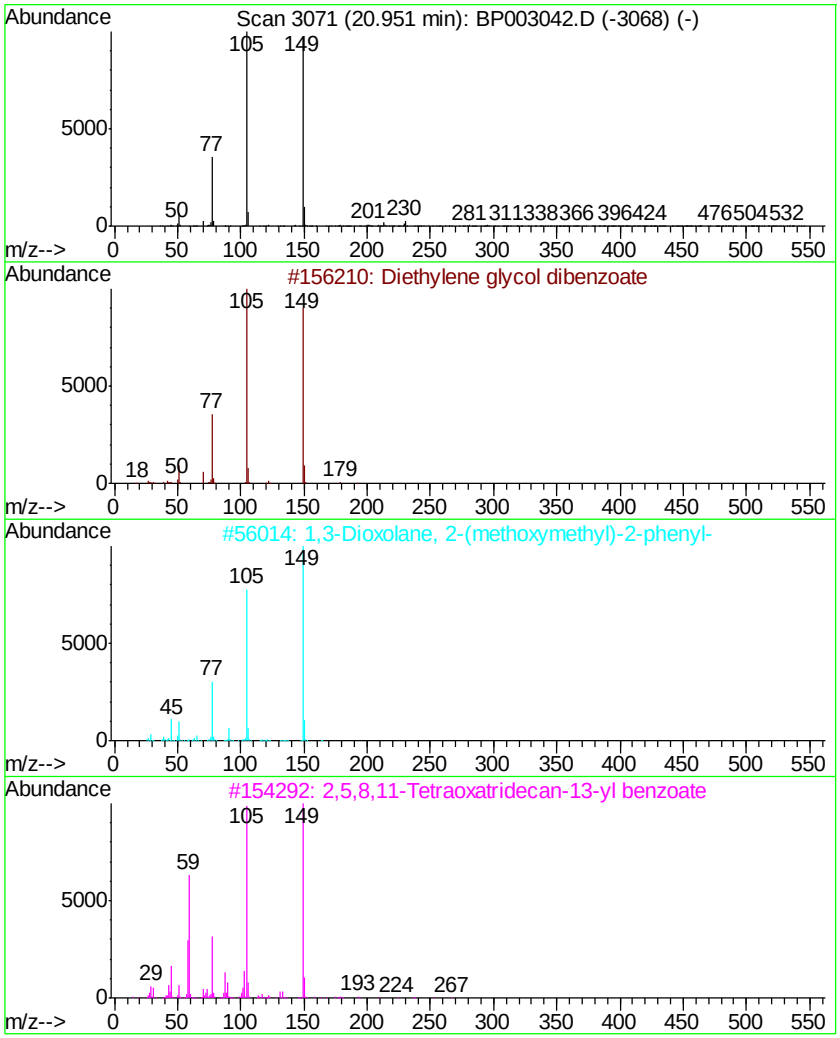
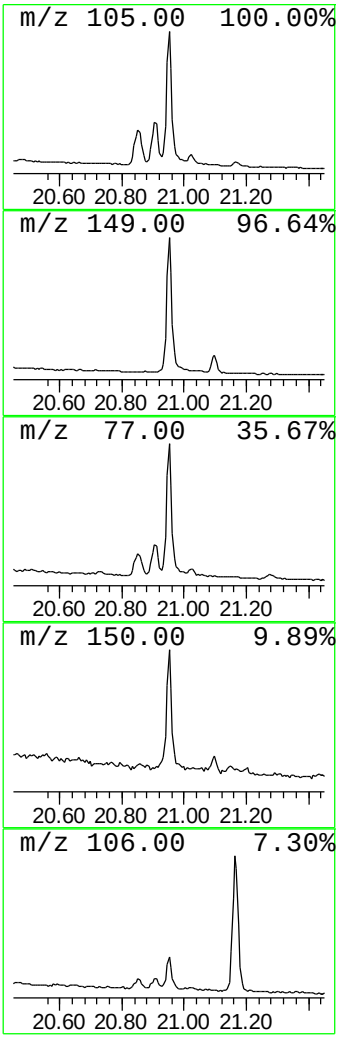
Peak Number 11 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	6.18 ng	1208970	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	78
3	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	78
4	2-(2-(2-Butoxyethoxy)ethoxy)ethy...	310	C17H26O5	1000366-97-2	64
5	Ethanol, 2-(4-phenoxyphenoxy)-, ...	334	C21H18O4	055191-59-8	50





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Instrument : BNA_P
ClientSampleId : CHRT-25433

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TIC Library : C:\DATABASE\NIST11.L
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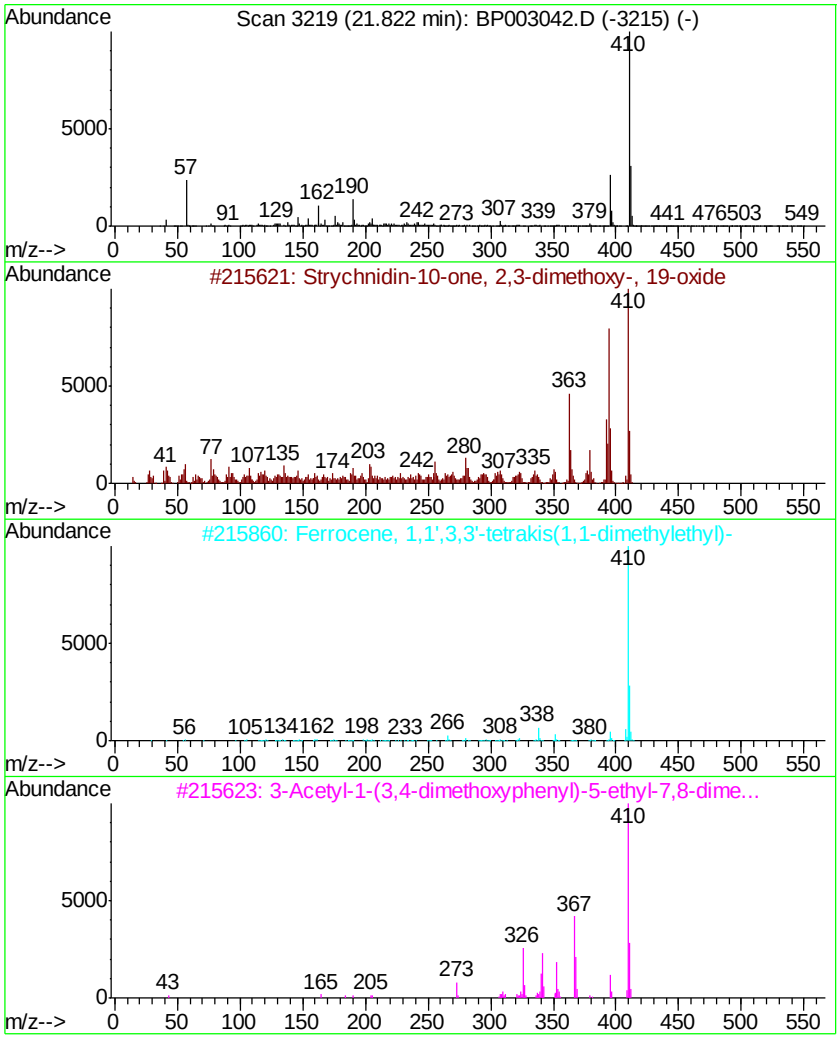
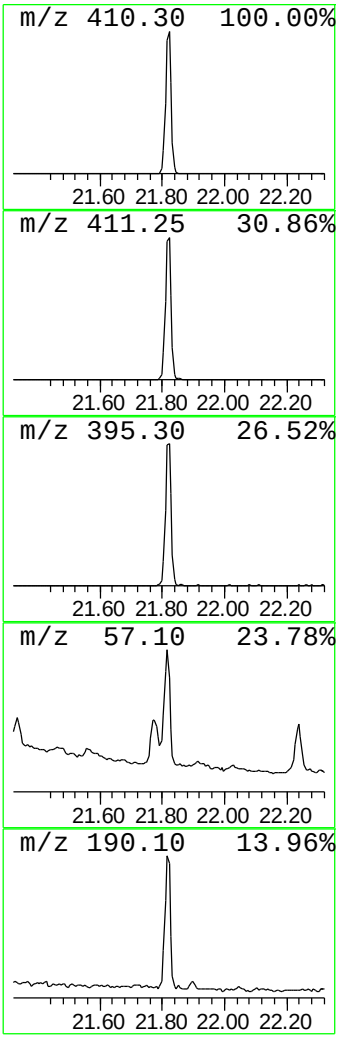
Peak Number 12 Strychnidin-10-one, 2,3-dim... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.82	5.15 ng	1006990	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Strychnidin-10-one, 2,3-dimethox...	410	C23H26N2O5	017301-81-4	72
2	Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	58
3	3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	42
4	6,9-Methanobenzo[h]pentaphene-5,...	410	C27H22O4	057427-50-6	40
5	Stigmasta-4,6,22-trien-3.beta.-ol	410	C29H46O	096737-58-5	38





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Operator : CG/JU
Sample : L3712-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.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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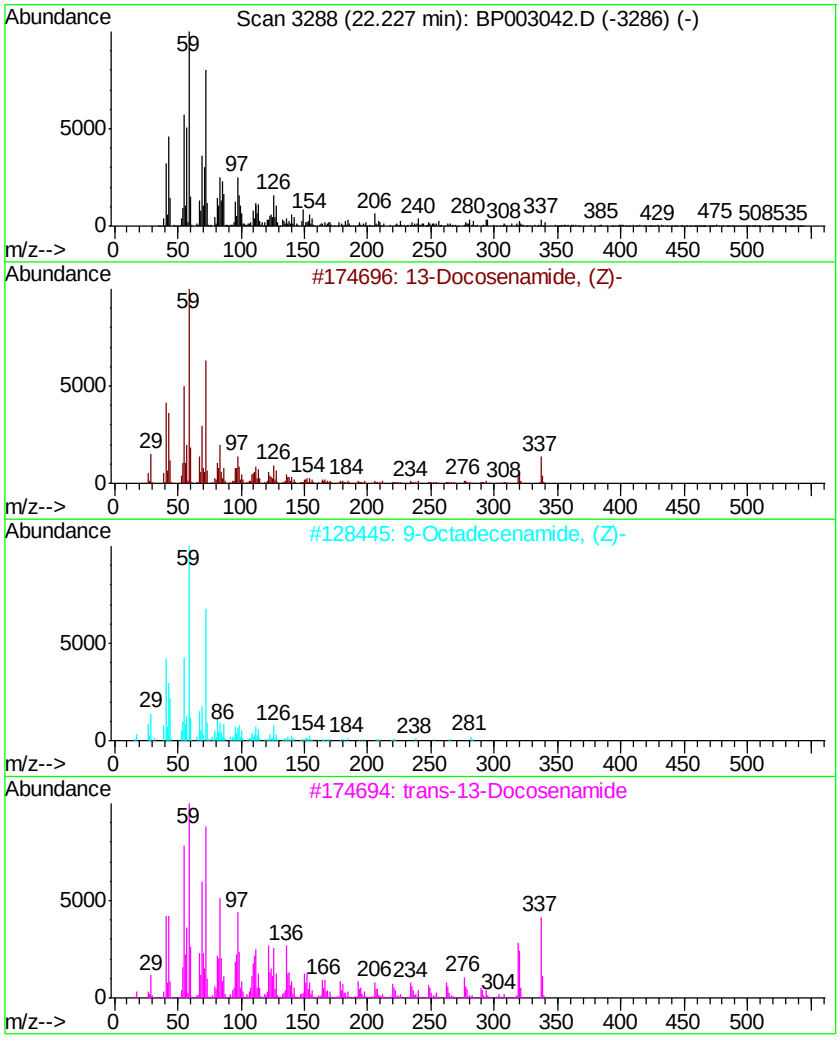
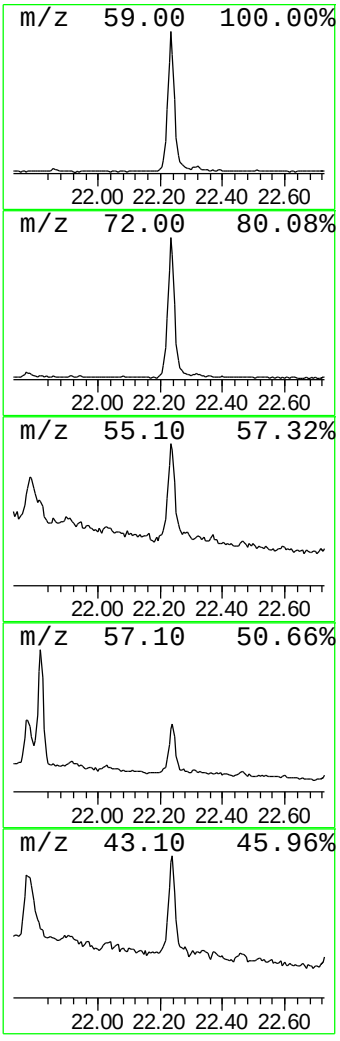
Peak Number 13 13-Docosenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.23	4.14 ng	810758	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	86
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	62
3	trans-13-Docosenamide	337	C22H43NO	010436-09-6	42
4	3-Dodecanone	184	C12H24O	001534-27-6	38
5	Octane, 1-(1-methoxyethoxy)-	188	C11H24O2	054789-26-3	35





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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

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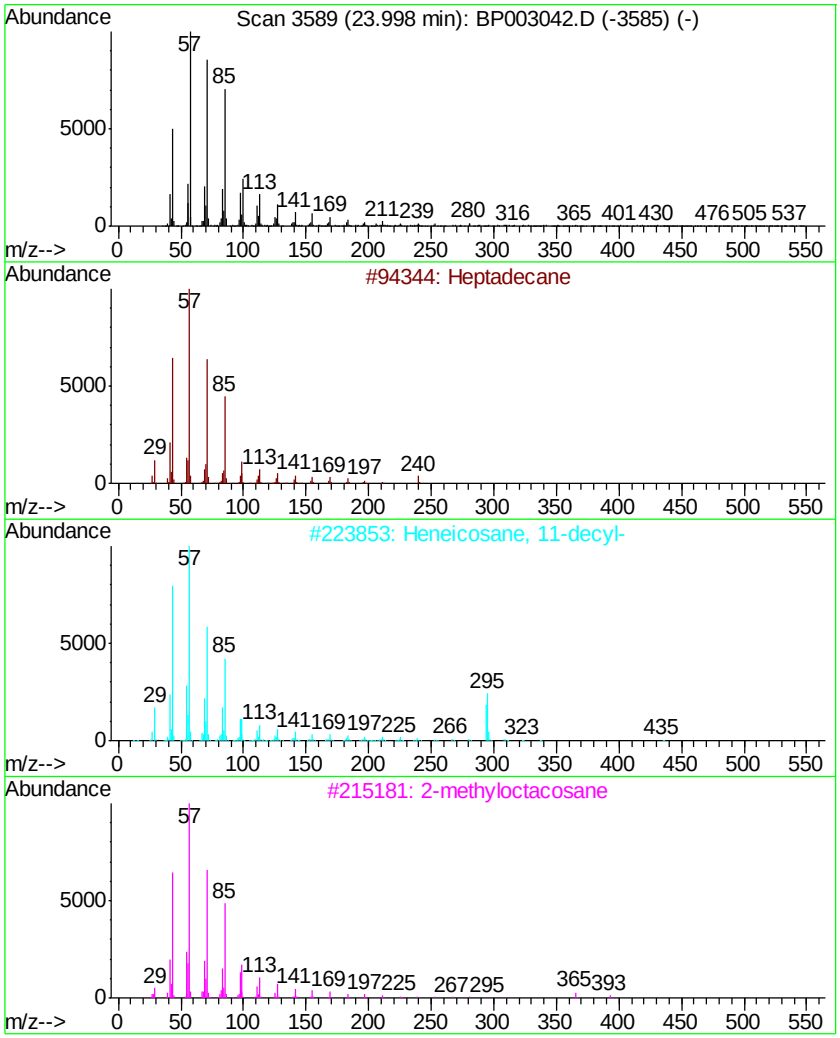
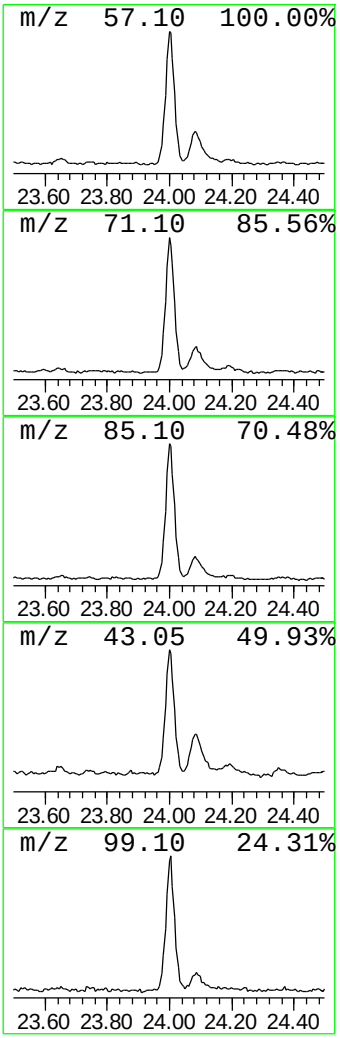
Peak Number 14 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	3.15 ng	776396	Perylene-d12	23.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	94
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Triacontane, 1-bromo-	500	C30H61Br	004209-22-7	91





Tentatively Identified Compound (LSC) summary

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Data File : BP003042.D
Acq On : 19 Aug 2020 20:37
Operator : CG/JU
Sample : L3712-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-25433

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.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
Butane, 2-methoxy...	2.95	18.0	ng	1598050	1	7.68	1777620	20.0
D-Limonene	7.92	2.3	ng	204558	1	7.68	1777620	20.0
unknown11.95	11.95	2.2	ng	293420	2	10.46	2712340	20.0
2-Pentanone, 4-cy...	13.12	2.9	ng	753372	3	14.32	5236710	20.0
Phenol, 2,6-bis(1...	13.68	5.6	ng	1469230	3	14.32	5236710	20.0
Decahydro-4,4,8,9...	14.16	8.3	ng	2168790	3	14.32	5236710	20.0
unknown14.24	14.24	2.4	ng	640005	3	14.32	5236710	20.0
Naphthalene, 1,2,...	14.66	3.0	ng	792983	3	14.32	5236710	20.0
unknown15.13	15.13	9.8	ng	2576850	3	14.32	5236710	20.0
5-Eicosene, (E)-	20.90	7.8	ng	1525000	5	21.16	3912280	20.0
Diethylene glycol...	20.95	6.2	ng	1208970	5	21.16	3912280	20.0
Strychnidin-10-on...	21.82	5.2	ng	1006990	5	21.16	3912280	20.0
13-Docosenamide, ...	22.23	4.1	ng	810758	5	21.16	3912280	20.0
Heptadecane	24.00	3.1	ng	776396	6	23.40	4926160	20.0