LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
Data File : BP009428.D
Acq On : 16 Mar 2022 18:19
Operator : CG/JU
Sample : N1951-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DB-14-(13-15)-3-12-22

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\8270E-BP030522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009428.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.052	7	11	27	rVB	425592	692995	4.32%	0.704%
2	5.416	406	413	433	rBV	5904007	9714086	60.62%	9.867%
3	7.005	669	683	698	rBV	5719289	10062913	62.80%	10.221%
4	7.805	812	819	829	rBV	1409176	2450929	15.30%	2.490%
5	8.963	1009	1016	1030	rVB	3752981	6737800	42.05%	6.844%
6	9.787	1150	1156	1163	rBV3	156100	301842	1.88%	0.307%
7	10.604	1285	1295	1305	rBV	1885740	3883928	24.24%	3.945%
8	11.104	1375	1380	1387	rVB2	307972	505813	3.16%	0.514%
9	11.293	1409	1412	1420	rVB9	164970	371570	2.32%	0.377%
10	11.381	1421	1427	1433	rBV10	102709	314160	1.96%	0.319%
11	11.681	1471	1478	1492	rVB8	231327	874868	5.46%	0.889%
12	11.798	1493	1498	1503	rBV	246435	418257	2.61%	0.425%
13	11.904	1511	1516	1521	rBV2	275492	494313	3.08%	0.502%
14	12.075	1536	1545	1551	rBV10	136378	486116	3.03%	0.494%
15	12.351	1587	1592	1599	rBV6	218855	564964	3.53%	0.574%
16	12.892	1681	1684	1689	rVB4	340802	518253	3.23%	0.526%
17	13.075	1708	1715	1725	rVB	9706629	16023288	100.00%	16.276%
18	13.240	1739	1743	1746	rBV	505548	826926	5.16%	0.840%
19	13.875	1847	1851	1858	rBV2	991989	1532090	9.56%	1.556%
20	14.287	1917	1921	1929	rVB3	1035940	2043195	12.75%	2.075%
21	14.451	1940	1949	1957	rBV	3311345	6572557	41.02%	6.676%
22	15.951	2198	2204	2211	rBV	7907511	12811711	79.96%	13.013%
23	17.216	2415	2419	2429	rVB	3190268	5029955	31.39%	5.109%
24	19.792	2853	2857	2862	rVB	12437311	15217312	94.97%	15.457%

Sum of corrected areas: 98449841

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
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Acq On : 16 Mar 2022 18:19
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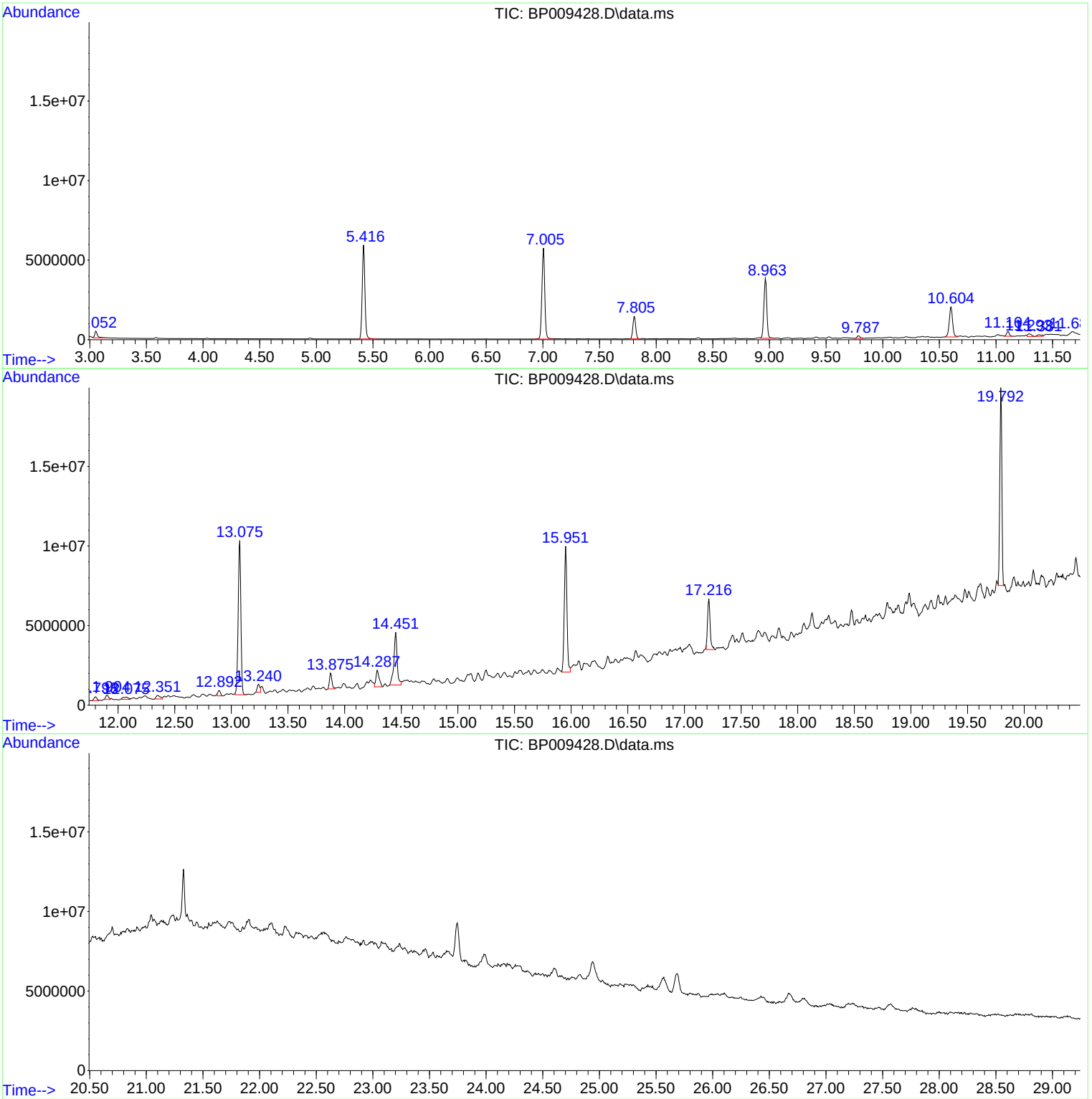
Sample : N1951-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DB-14-(13-15)-3-12-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Data File : BP009428.D
Acq On : 16 Mar 2022 18:19
Operator : CG/JU
Sample : N1951-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

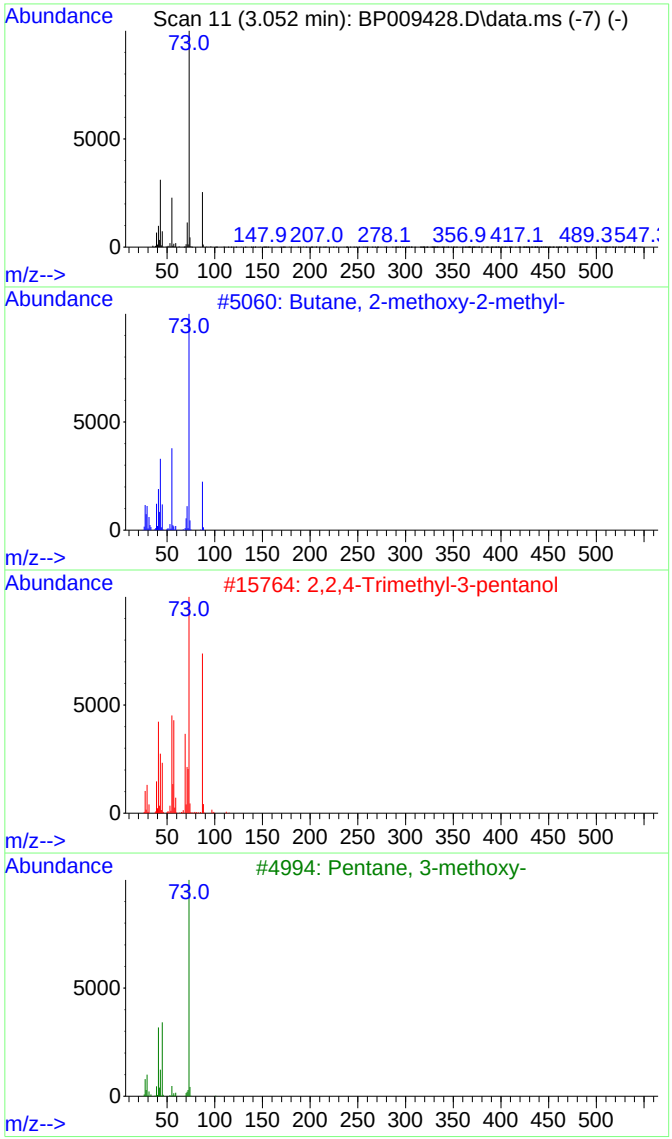
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

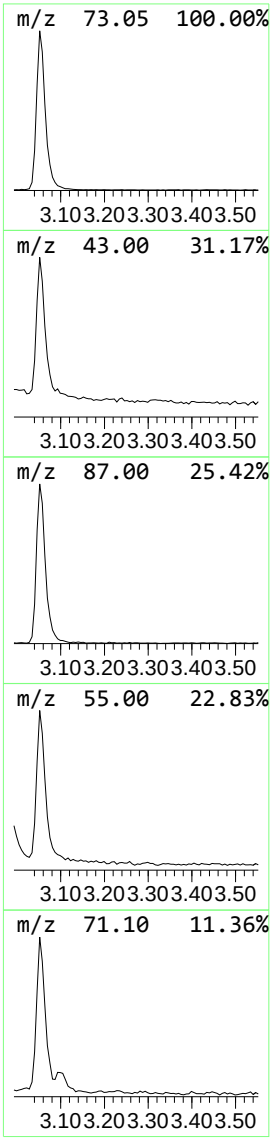
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.052	5.65 ng	692995	1,4-Dichlorobenzene-d4	7.805

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
Data File : BP009428.D
Acq On : 16 Mar 2022 18:19
Operator : CG/JU
Sample : N1951-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DB-14-(13-15)-3-12-22

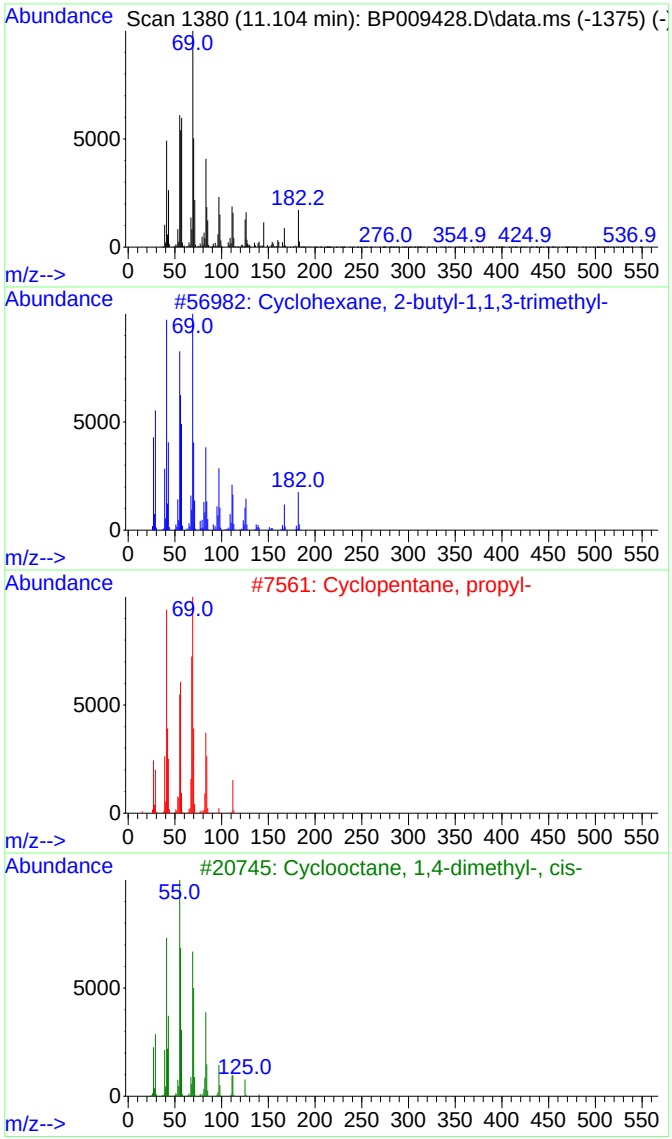
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

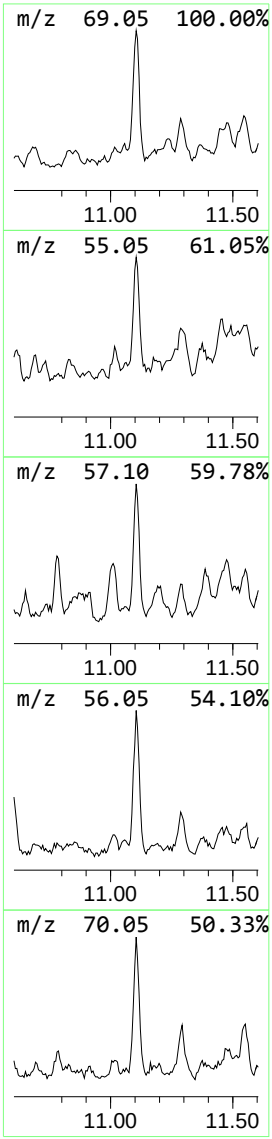
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, 2-butyl-1,1,3-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.104	2.60 ng	505813	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 2-butyl-1,1,3-trime...	182	C13H26	054676-39-0	96
2	Cyclopentane, propyl-	112	C8H16	002040-96-2	64
3	Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	60
4	2-Dodecene, 2-methyl-	182	C13H26	055103-82-7	52
5	Cyclobutane, 1-butyl-2-ethyl-	140	C10H20	1010150-67-3	50





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Data File : BP009428.D
Acq On : 16 Mar 2022 18:19
Operator : CG/JU
Sample : N1951-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DB-14-(13-15)-3-12-22

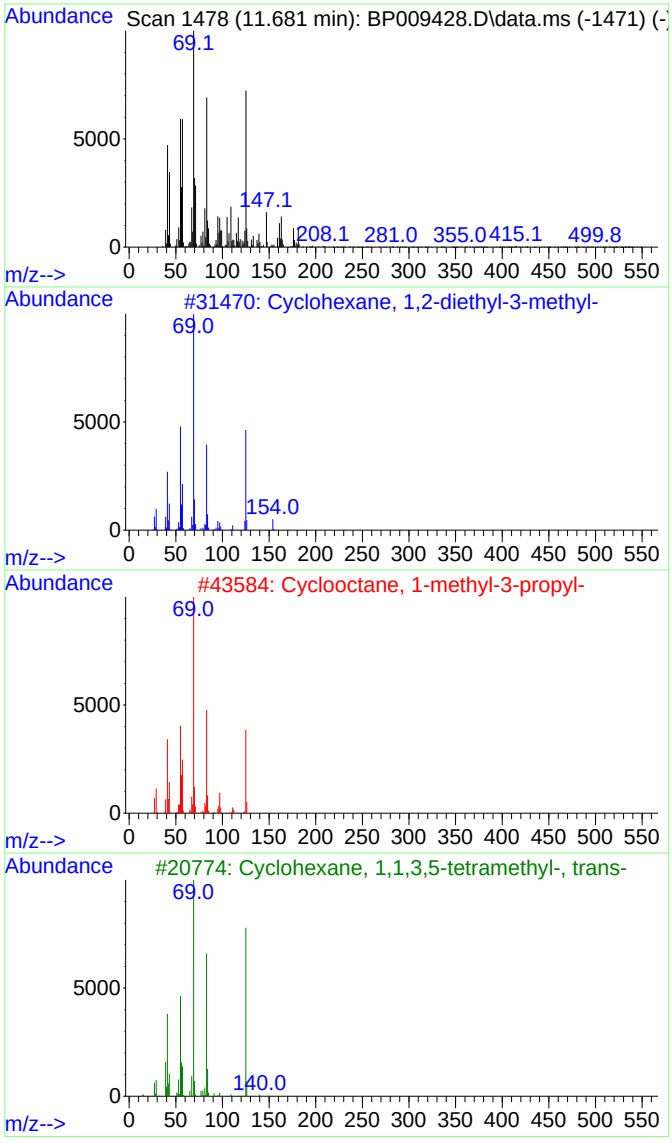
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

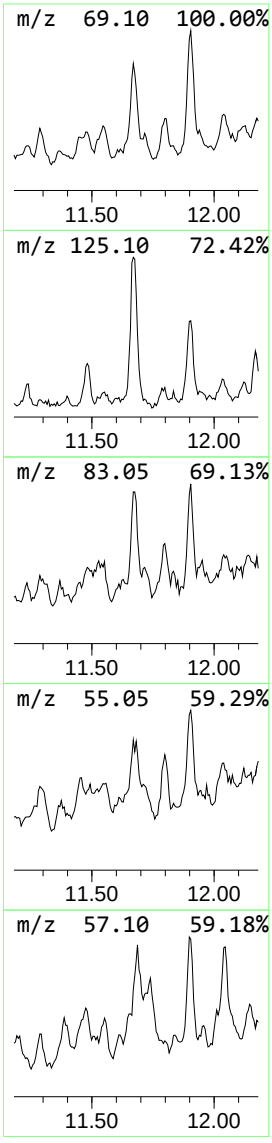
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, 1,2-diethyl-3-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.681	4.51 ng	874868	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-diethyl-3-methyl-	154	C11H22	061141-80-8	53
2	Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	53
3	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	53
4	Cyclohexane, 1,1,4,4-tetramethyl-	140	C10H20	002223-52-1	49
5	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
Data File : BP009428.D
Acq On : 16 Mar 2022 18:19
Operator : CG/JU
Sample : N1951-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DB-14-(13-15)-3-12-22

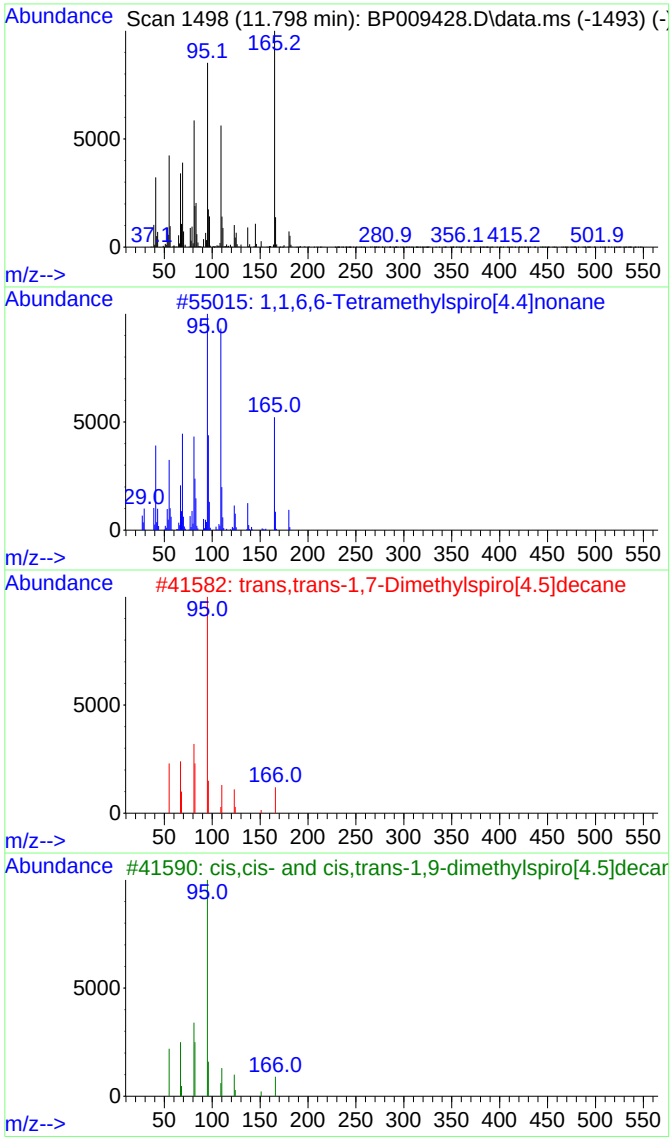
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

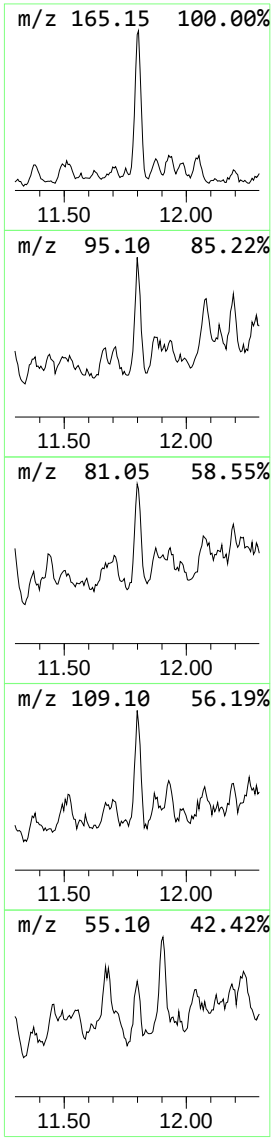
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1,1,6,6-Tetramethylspiro[4.... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.798	2.15 ng	418257	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,6,6-Tetramethylspiro[4.4]nonane	180	C13H24	074054-92-5	58
2	trans,trans-1,7-Dimethylspiro[4....	166	C12H22	1000111-72-6	41
3	cis,cis- and cis,trans-1,9-dimet...	166	C12H22	1000111-72-5	38
4	trans,cis-1,7-Dimethylspiro[4.5]...	166	C12H22	1010111-72-7	38
5	1,5-Dihydro-1,5-dimethyl-6H-imid...	165	C6H7N5O	106284-73-5	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
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Acq On : 16 Mar 2022 18:19
Operator : CG/JU
Sample : N1951-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DB-14-(13-15)-3-12-22

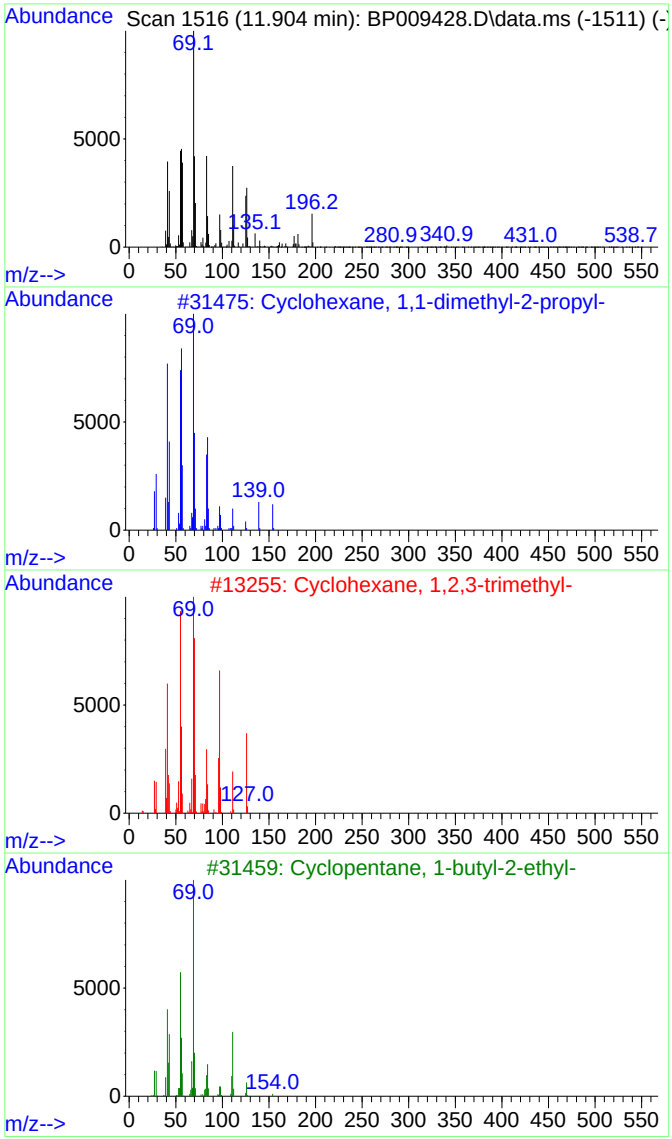
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

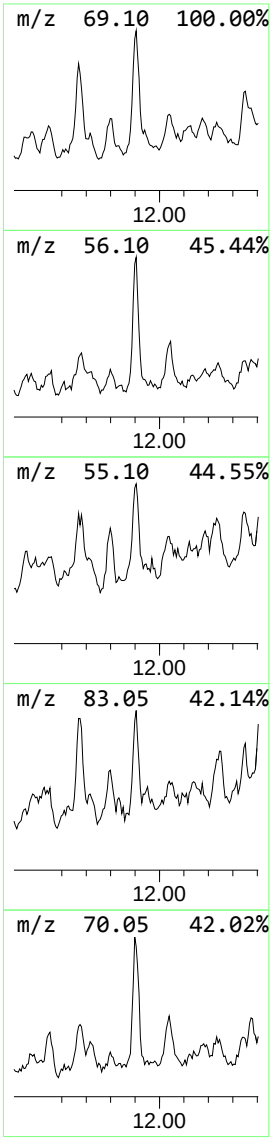
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexane, 1,1-dimethyl-2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	2.55 ng	494313	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1-dimethyl-2-propyl-	154	C11H22	081983-71-3	59
2	Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	50
3	Cyclopentane, 1-butyl-2-ethyl-	154	C11H22	072993-32-9	47
4	Cyclohexanone, 3,5-dimethyl-	126	C8H14O	002320-30-1	47
5	3-Hexene, 2,5-dimethyl-	112	C8H16	015910-22-2	43





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Sample : N1951-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DB-14-(13-15)-3-12-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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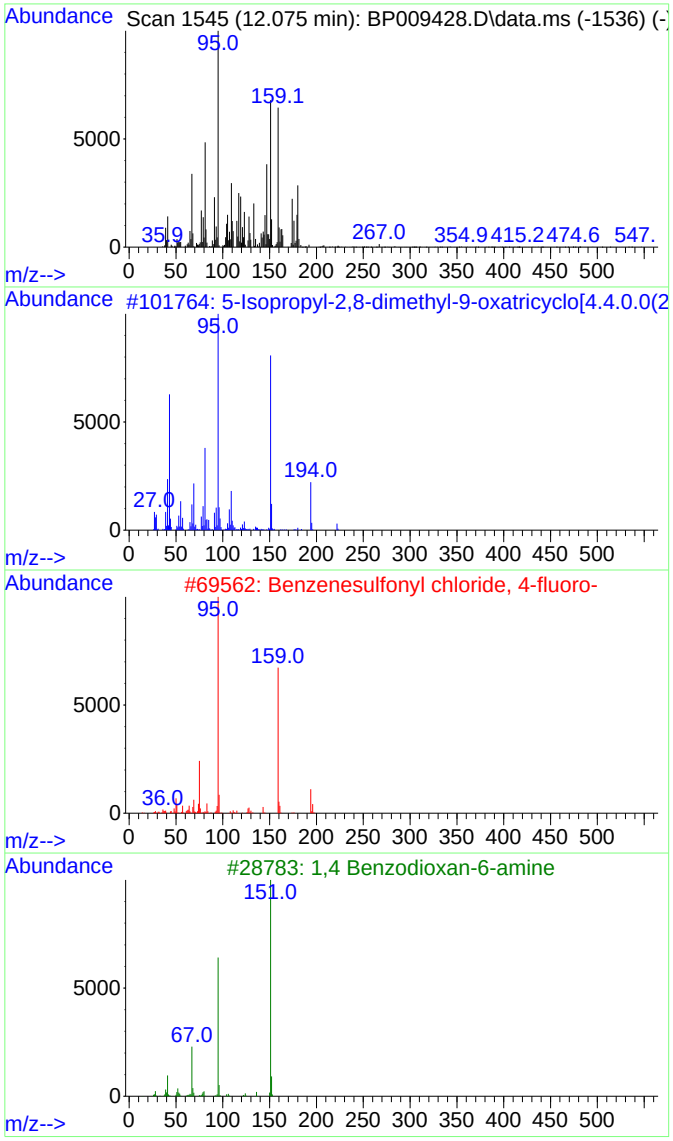
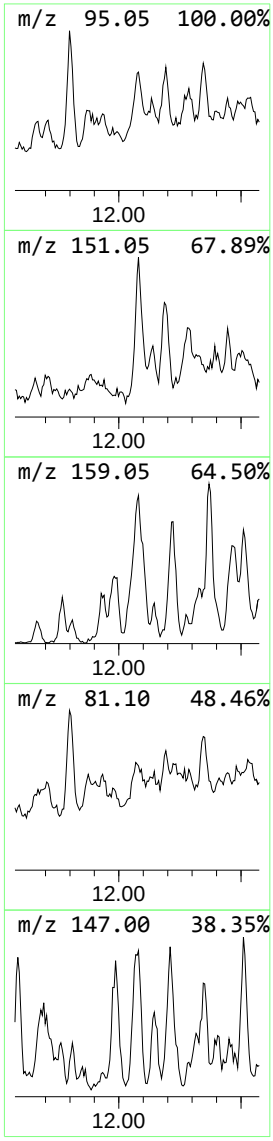
****

Peak Number 6 unknown12.075 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.075	2.50 ng	486116	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Isopropyl-2,8-dimethyl-9-oxatr...	222	C14H22O2	1010185-23-8	27
2	Benzenesulfonyl chloride, 4-fluoro-	194	C6H4ClFO2S	000349-88-2	22
3	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	22
4	2-Furancarboxamide, N-(2-phenyle...	271	C17H21NO2	1000451-26-7	14
5	(+)-2-Bornanone	152	C10H16O	000464-49-3	14





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BNA_P
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DB-14-(13-15)-3-12-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

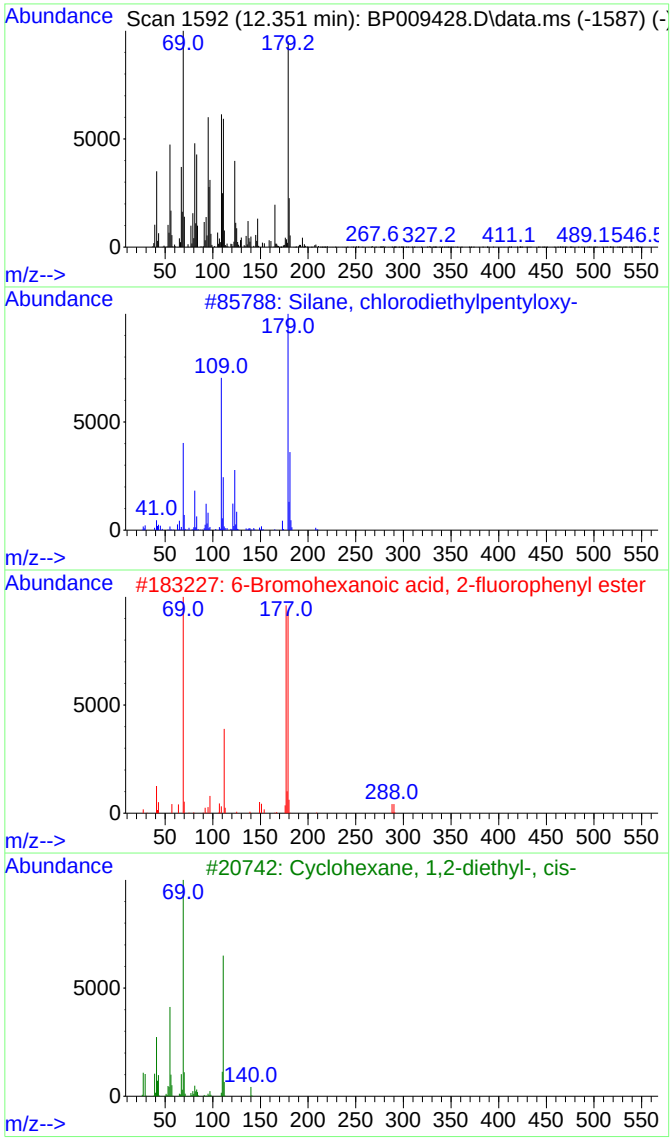
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

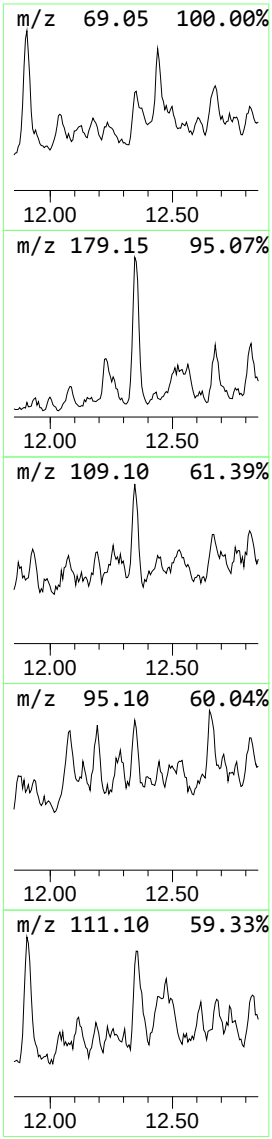
****

Peak Number 7 unknown12.351 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.351	2.91 ng	564964	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, chlorodiethylpentyloxy-	208	C9H21ClOSi	1000363-04-4	35
2	6-Bromohexanoic acid, 2-fluoroph...	288	C12H14BrFO2	1000325-75-5	27
3	Cyclohexane, 1,2-diethyl-, cis-	140	C10H20	000824-43-1	25
4	Cyclohexane, (1,2-dimethylbutyl)-	168	C12H24	061142-37-8	22
5	1,3-Dimethyl-(3,7-dimethyloctyl)...	252	C18H36	1000113-02-4	22





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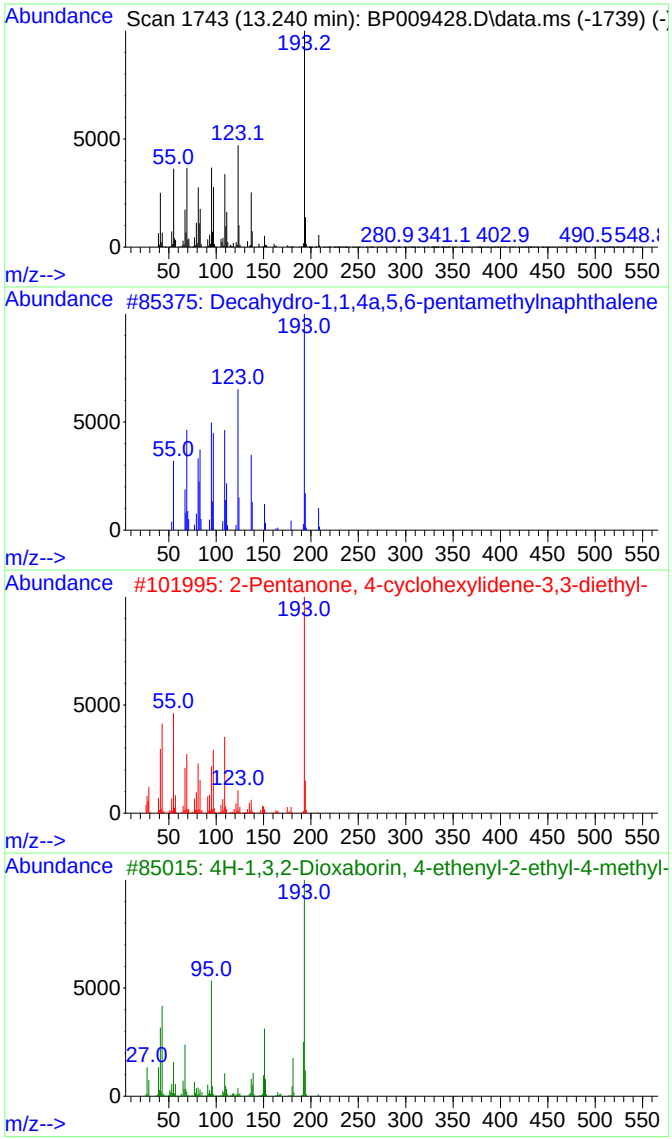
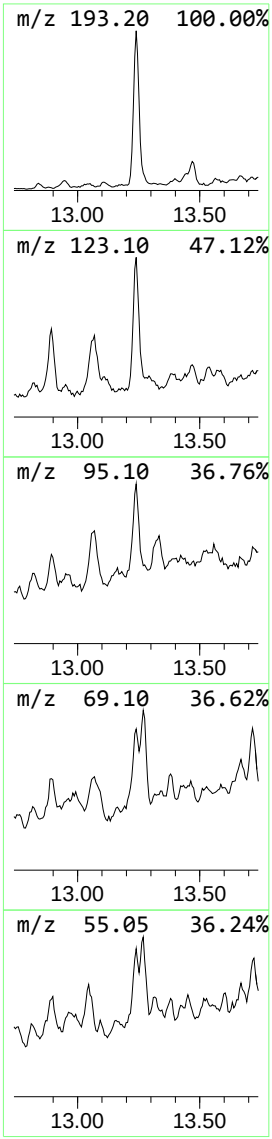
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.240	2.52 ng	826926	Acenaphthene-d10	14.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	90
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	38
3	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21BO2	074630-04-9	32
4	2-(1-Butyl-2-nitroallyl)cyclohex...	239	C13H21NO3	1000192-05-9	25
5	2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	25





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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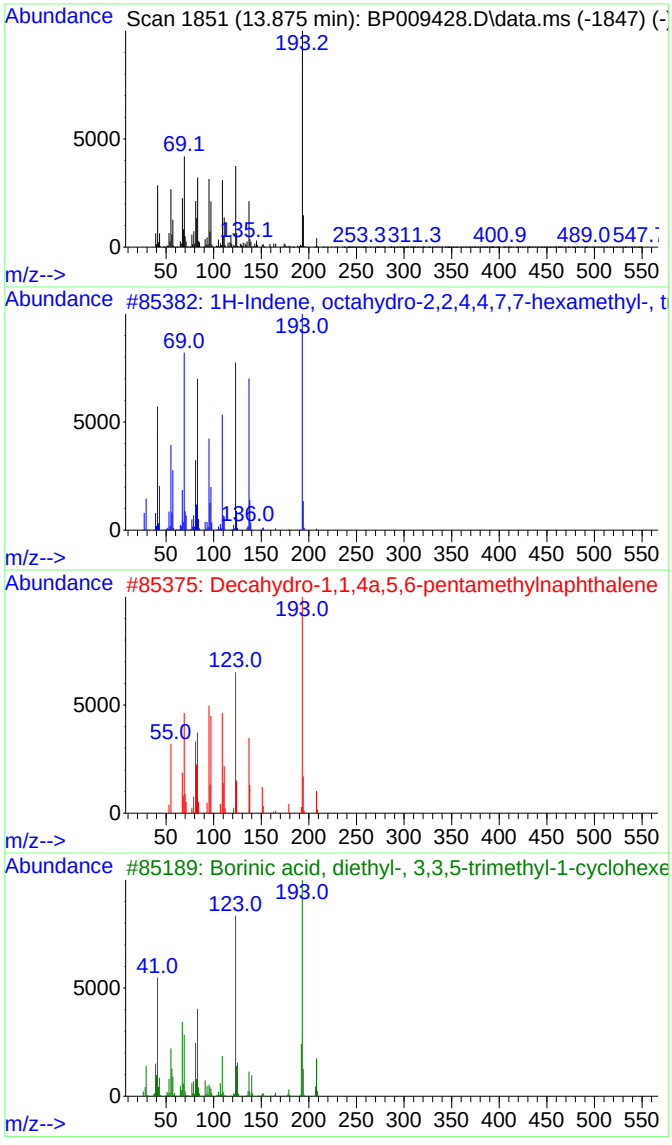
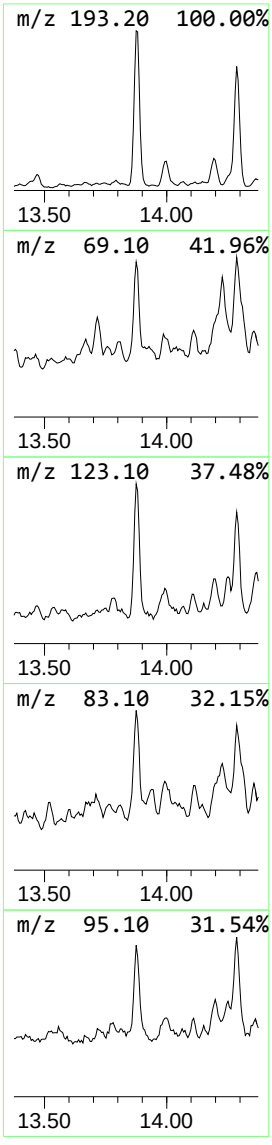
****

Peak Number 9 unknown13.875 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.875	4.66 ng	1532090	Acenaphthene-d10	14.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	45
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	43
3	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	38
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	37
5	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
Data File : BP009428.D
Acq On : 16 Mar 2022 18:19
Operator : CG/JU
Sample : N1951-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DB-14-(13-15)-3-12-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

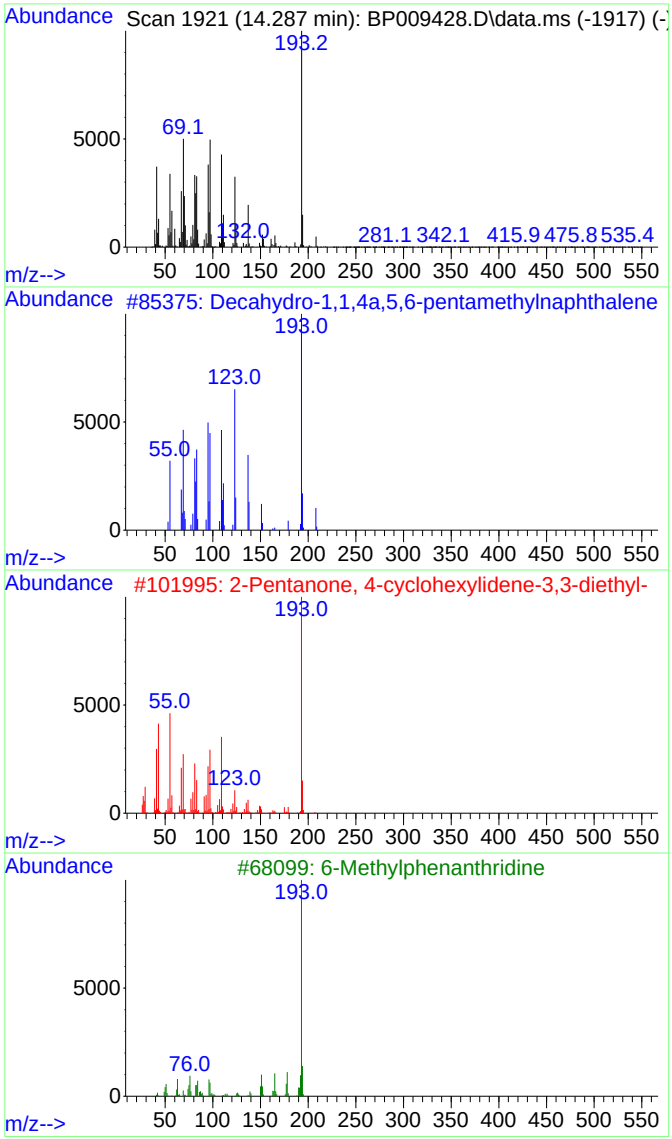
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

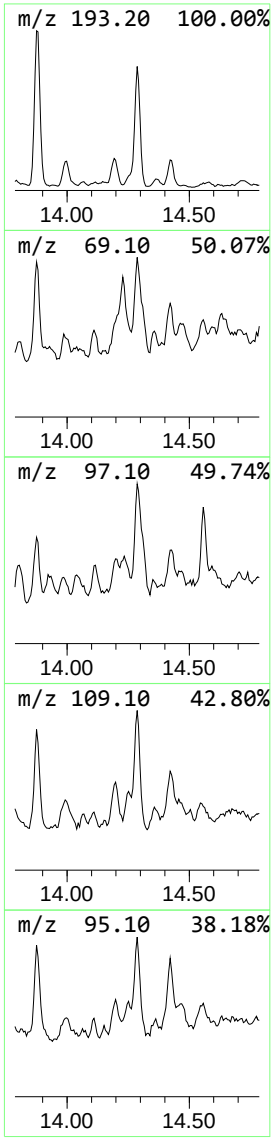
****

Peak Number 10 unknown14.287 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.287	6.22 ng	2043200	Acenaphthene-d10	14.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	47
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	33
3	6-Methylphenanthridine	193	C14H11N	003955-65-5	22
4	2-((Trimethylsilyl)thio)nicotino...	208	C9H12N2SSi	1000474-02-5	22
5	2-Anthracenamine	193	C14H11N	000613-13-8	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
Data File : BP009428.D
Acq On : 16 Mar 2022 18:19
Operator : CG/JU
Sample : N1951-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DB-14-(13-15)-3-12-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.052	5.7	ng	692995	1	7.805	2450930	20.0
Cyclohexane, 2-...	11.104	2.6	ng	505813	2	10.604	3883930	20.0
Cyclohexane, 1,...	11.681	4.5	ng	874868	2	10.604	3883930	20.0
1,1,6,6-Tetrame...	11.798	2.1	ng	418257	2	10.604	3883930	20.0
Cyclohexane, 1,...	11.904	2.5	ng	494313	2	10.604	3883930	20.0
unknown12.075	12.075	2.5	ng	486116	2	10.604	3883930	20.0
unknown12.351	12.351	2.9	ng	564964	2	10.604	3883930	20.0
Decahydro-1,1,4...	13.240	2.5	ng	826926	3	14.451	6572560	20.0
unknown13.875	13.875	4.7	ng	1532090	3	14.451	6572560	20.0
unknown14.287	14.287	6.2	ng	2043200	3	14.451	6572560	20.0