LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134394.D
Acq On : 21 Jul 2023 11:08
Operator : CG\JU
Sample : 03630-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-303-20230713

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134394.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	9	rBV	848041	1234836	27.83%	6.636%
2	2.169	9	14	19	rVB	2928725	4436477	100.00%	23.843%
3	5.475	572	576	589	rBV	776244	791984	17.85%	4.256%
4	5.616	597	600	603	rBV	166876	138757	3.13%	0.746%
5	5.663	603	608	614	rVB	272708	243684	5.49%	1.310%
6	6.092	678	681	692	rBV	157790	140371	3.16%	0.754%
7	6.475	742	746	758	rBV	475193	477137	10.75%	2.564%
8	6.834	804	807	814	rBV	437888	366987	8.27%	1.972%
9	6.992	828	834	847	rVB2	210531	256899	5.79%	1.381%
10	7.404	899	904	907	rBV	1431757	1260455	28.41%	6.774%
11	7.969	997	1000	1017	rVB	70132	118005	2.66%	0.634%
12	8.116	1021	1025	1028	rBV	584831	469536	10.58%	2.523%
13	9.192	1204	1208	1211	rBV	2887576	2400568	54.11%	12.901%
14	9.875	1320	1324	1327	rBV	657677	537827	12.12%	2.890%
15	10.669	1455	1459	1468	rBV	1736809	1573264	35.46%	8.455%
16	11.369	1574	1578	1586	rBV	699517	562616	12.68%	3.024%
17	11.892	1663	1667	1678	rBV2	97198	115670	2.61%	0.622%
18	12.969	1845	1850	1853	rBV	2915183	2601577	58.64%	13.981%
19	14.033	2027	2031	2039	rVB	470650	463103	10.44%	2.489%
20	15.539	2281	2287	2298	rBV	304211	417580	9.41%	2.244%

Sum of corrected areas: 18607333

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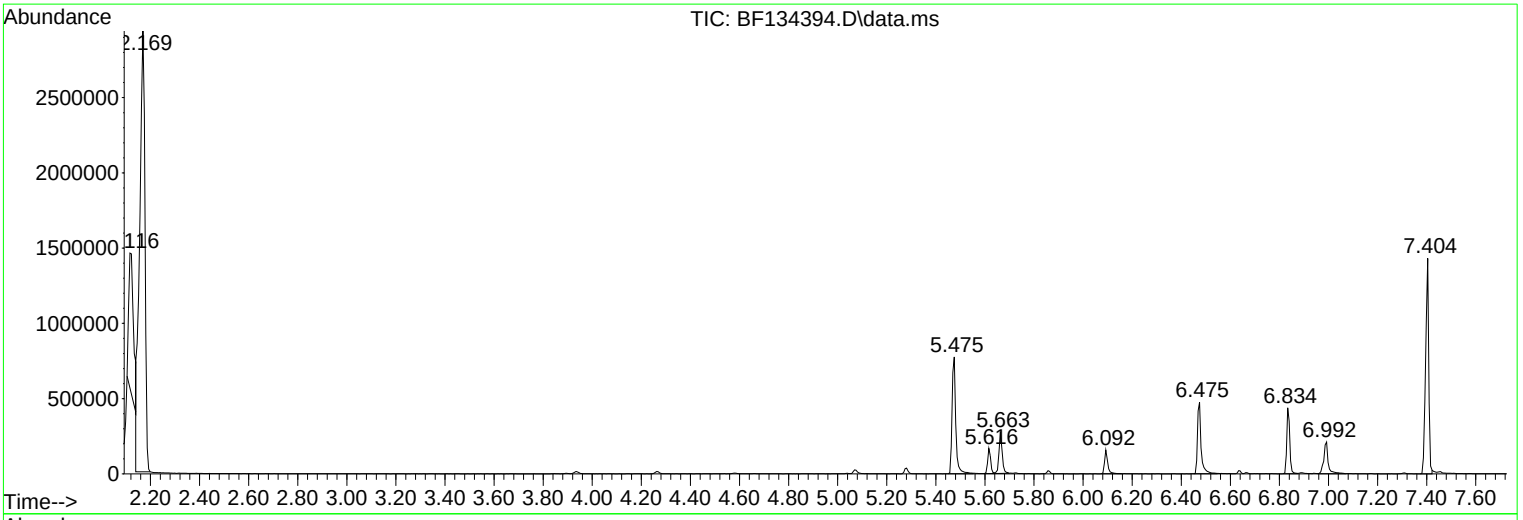
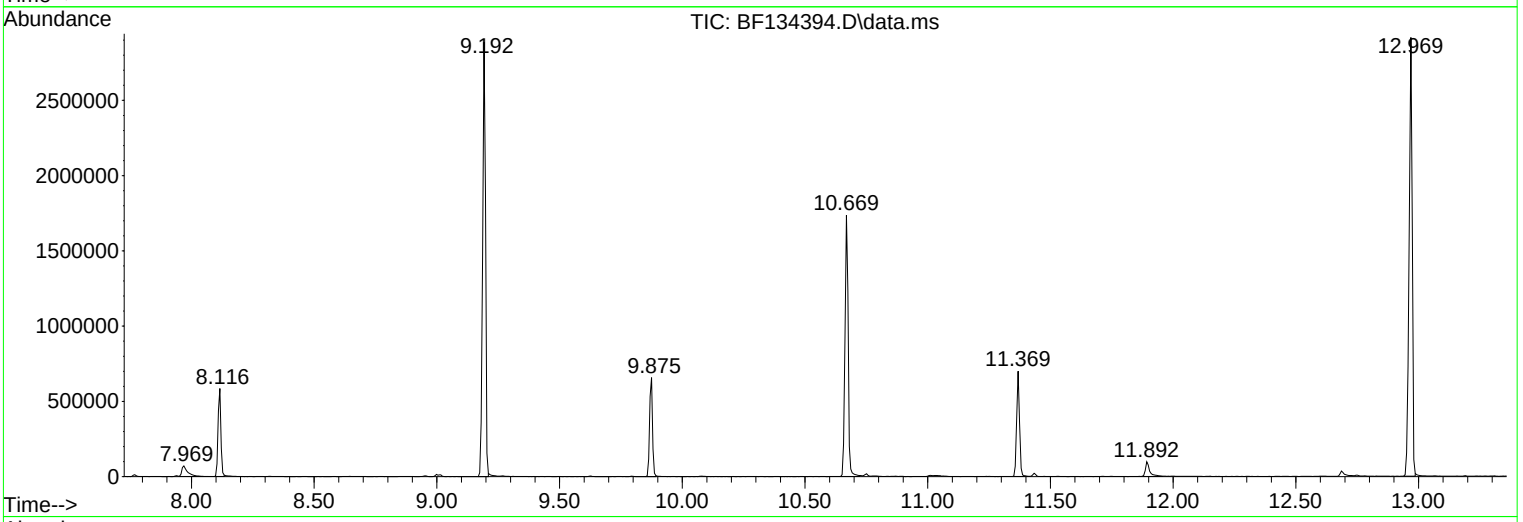
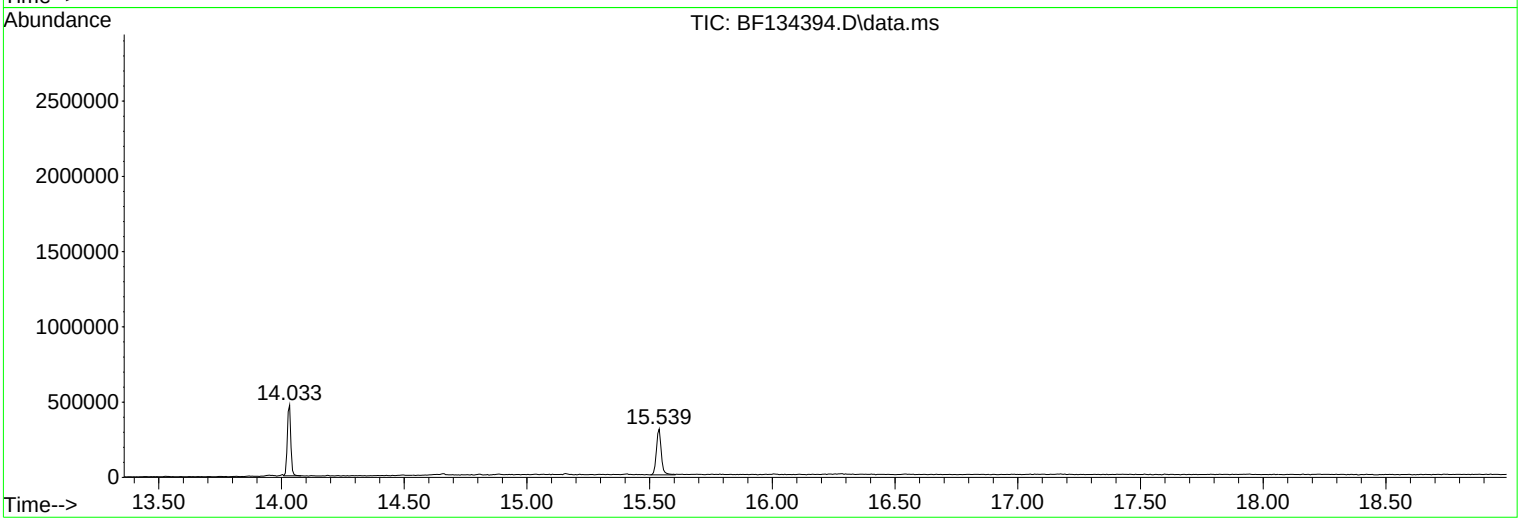
BNA_F
ClientSampleId :
SP-303-20230713

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

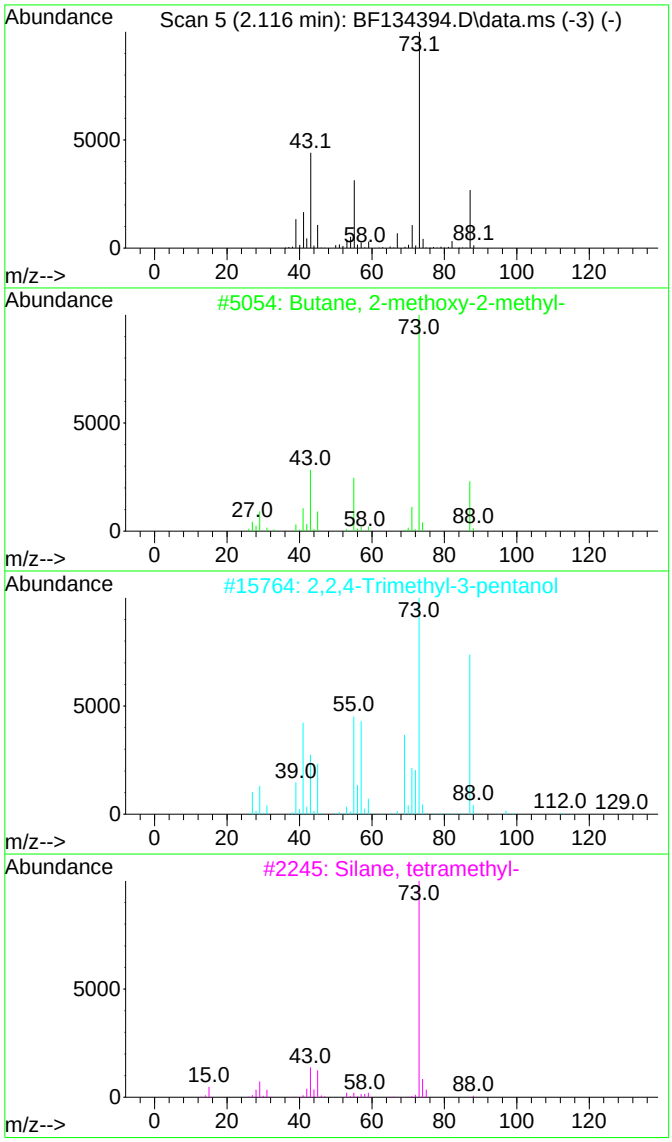
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

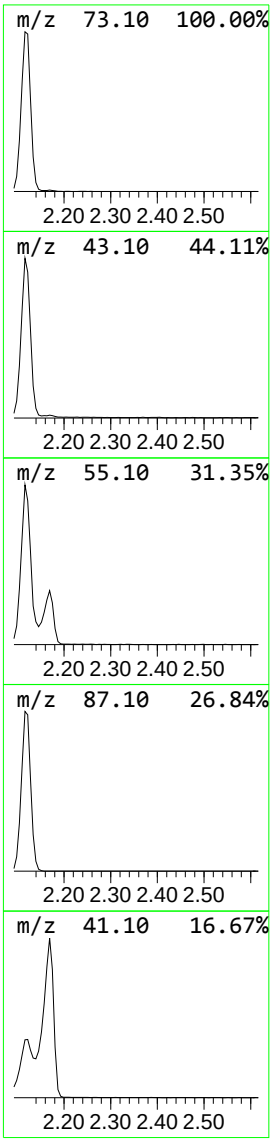
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	67.30 ng	1234840	1,4-Dichlorobenzene-d4	6.834

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Sample : 03630-03
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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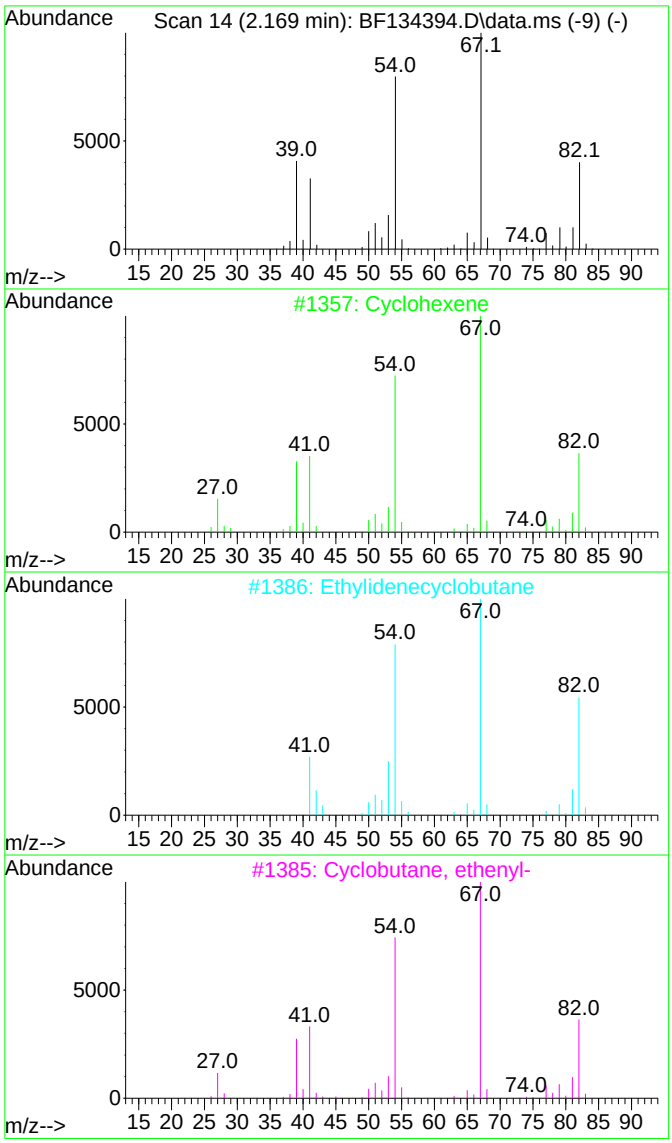
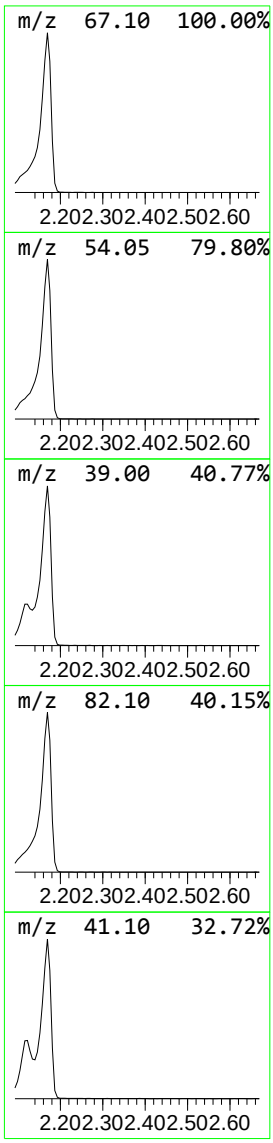
Peak Number 2 Cyclohexene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	241.78 ng	4436480	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene	82	C6H10	000110-83-8	93
2	Ethylidenecyclobutane	82	C6H10	001528-21-8	91
3	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	90
4	1,3-Pentadiene, 2-methyl-	82	C6H10	001118-58-7	38
5	2,4-Hexadiene, (E,E)-	82	C6H10	005194-51-4	38





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Operator : CG\JU
Sample : 03630-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-303-20230713

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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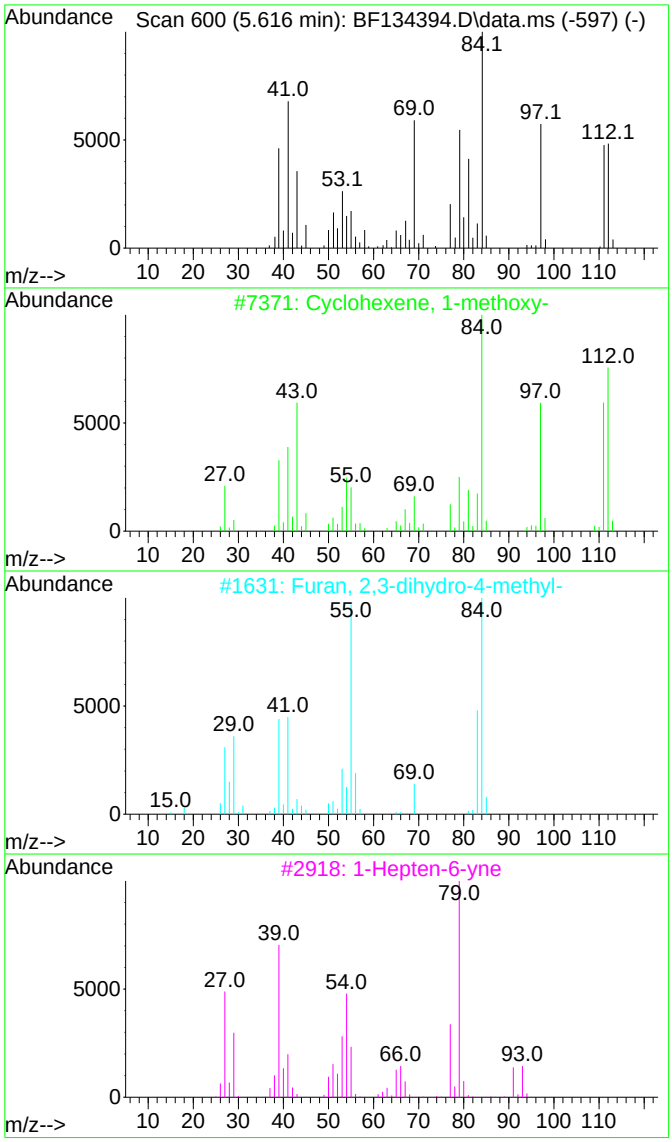
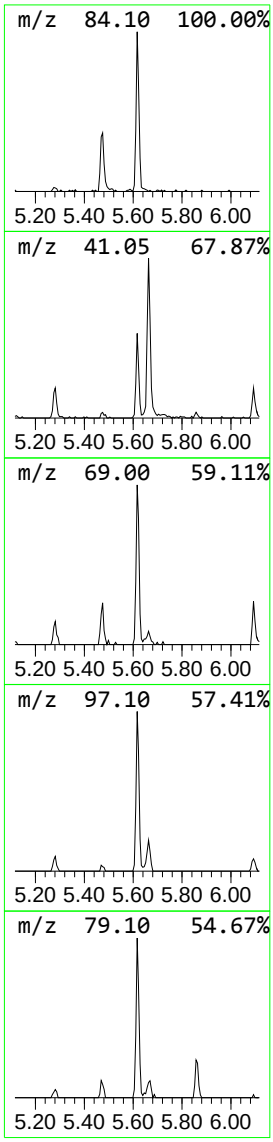
Peak Number 3 unknown5.616 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.616	7.56 ng	138757	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-methoxy-	112	C7H12O	000931-57-7	38
2	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	27
3	1-Hepten-6-yne	94	C7H10	065939-59-5	25
4	Thiophene, 2,3-dimethyl-	112	C6H8S	000632-16-6	22
5	Sorbic Acid	112	C6H8O2	000110-44-1	14





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Instrument :
BNA_F
ClientSampleId :
SP-303-20230713

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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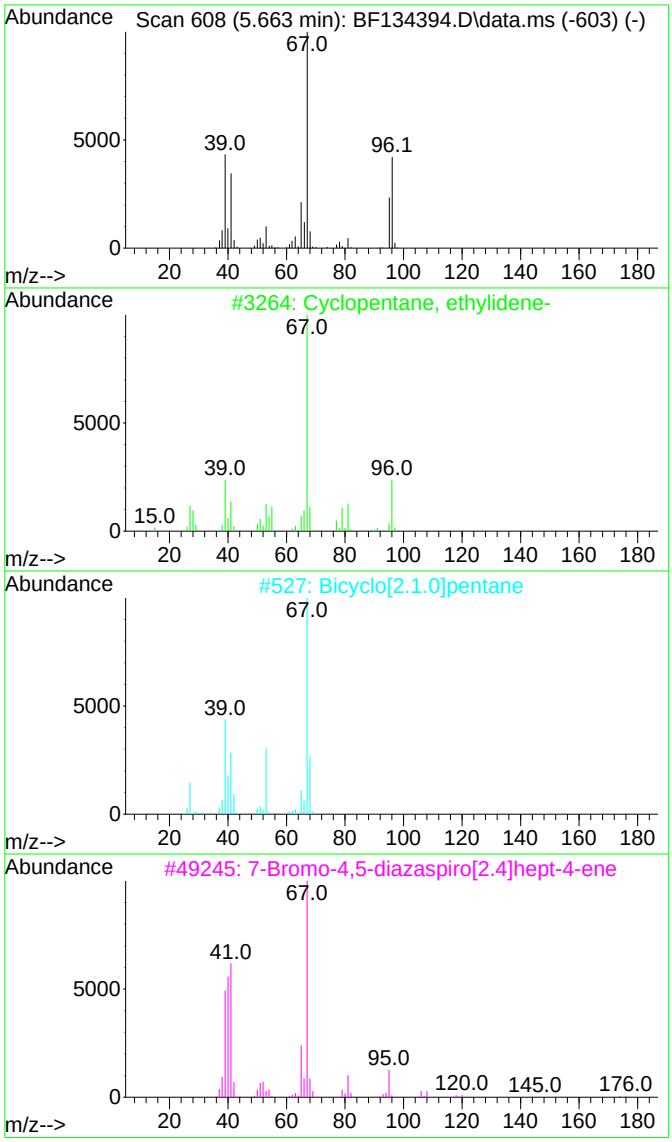
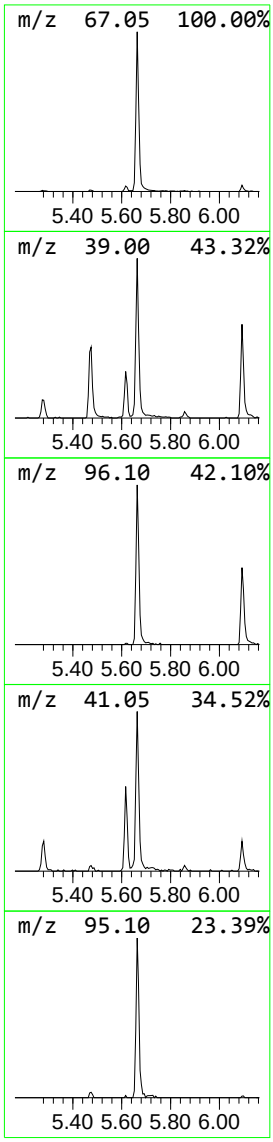
Peak Number 4 unknown5.663 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.663	13.28 ng	243684	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, ethylidene-	96	C7H12	002146-37-4	40
2	Bicyclo[2.1.0]pentane	68	C5H8	000185-94-4	40
3	7-Bromo-4,5-diazaspiro[2.4]hept-...	174	C5H7BrN2	1000261-52-7	36
4	1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	35
5	1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	35





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Misc :
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Instrument :
BNA_F
ClientSampleId :
SP-303-20230713

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

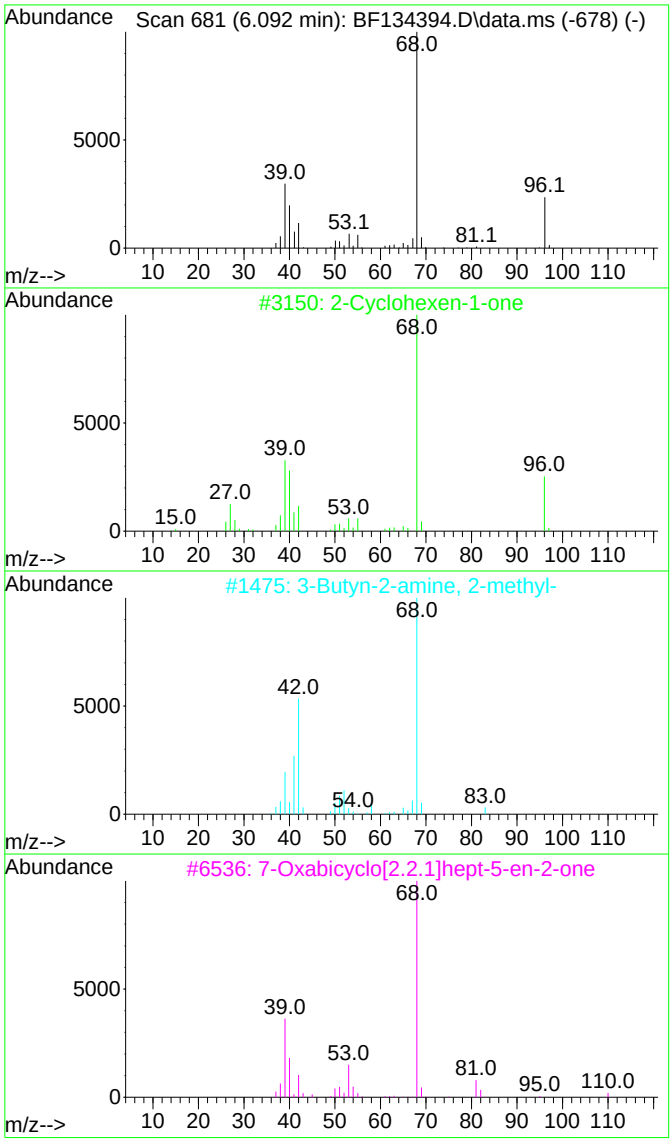
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

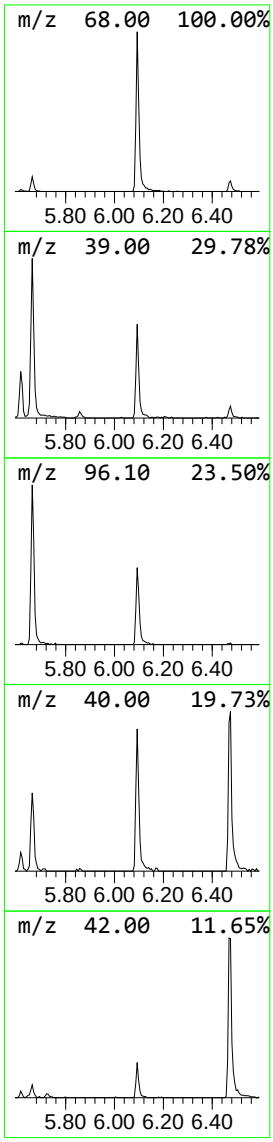
****

Peak Number 5 2-Cyclohexen-1-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.092	7.65 ng	140371	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	94
2	3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	59
3	7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	42
4	But-1-ene-3-yne, 1-ethoxy-	96	C6H8O	002806-41-9	14
5	1,5-Cyclooctadien-4-one	122	C8H10O	001460-21-5	12





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

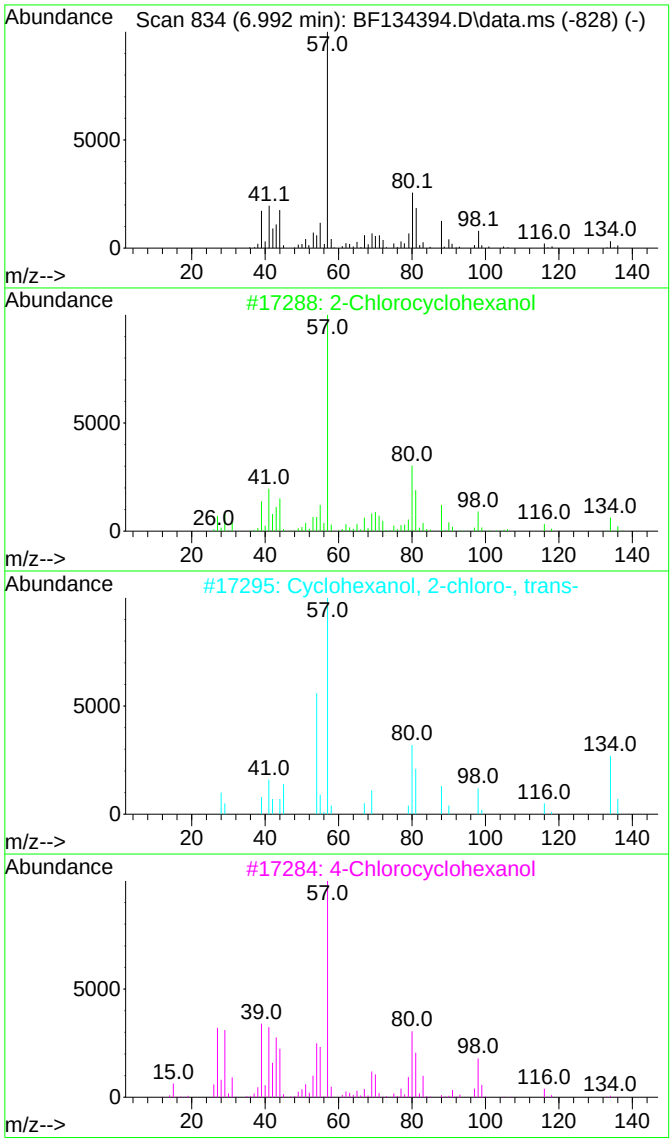
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

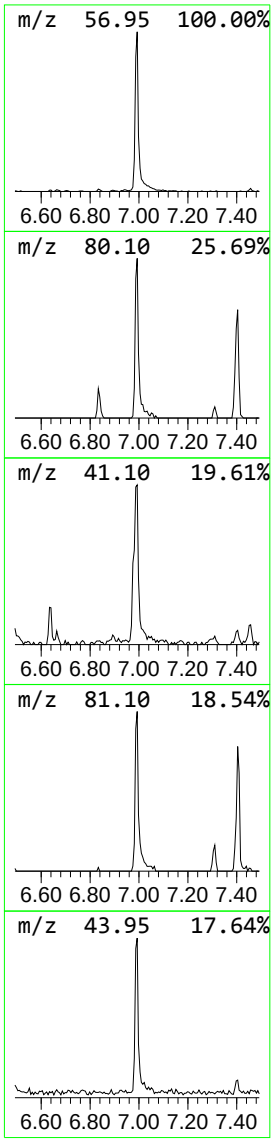
****

Peak Number 6 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.992	14.00 ng	256899	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	95
2	Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	43
3	4-Chlorocyclohexanol	134	C6H11ClO	030485-71-3	38
4	Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	37
5	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	14





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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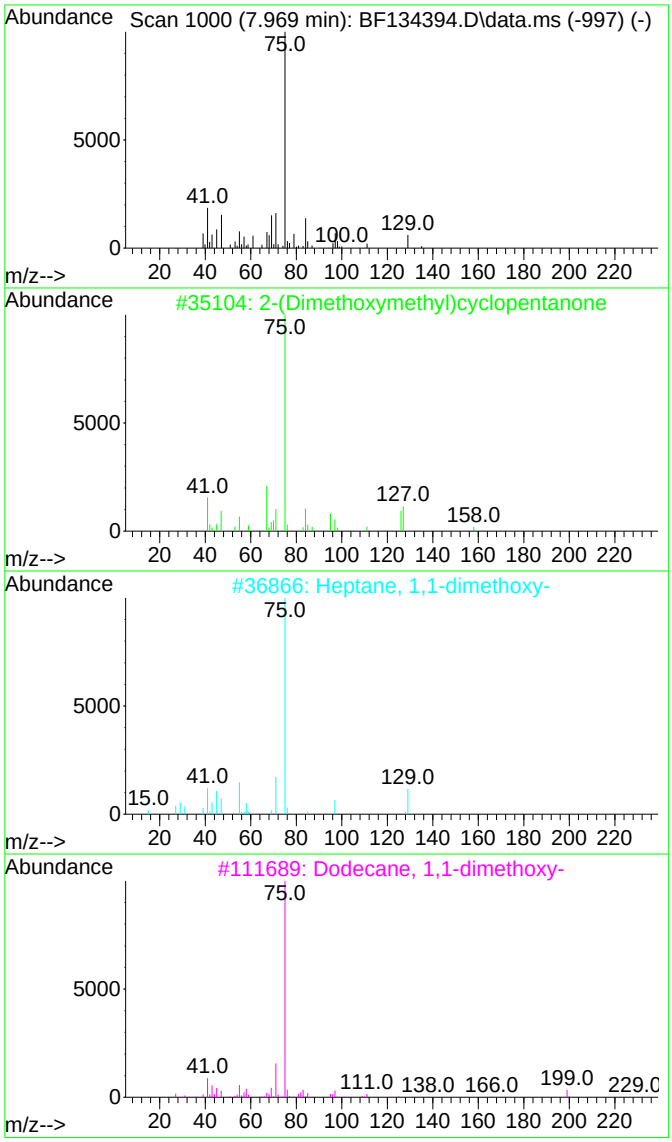
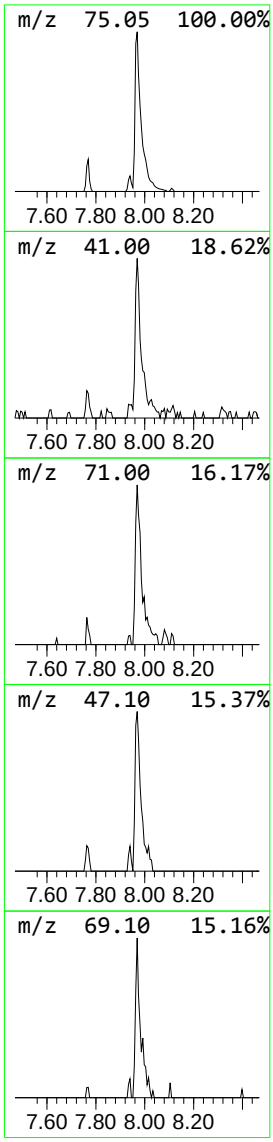
Peak Number 7 2-(Dimethoxymethyl)cyclopen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.969	5.03 ng	118005	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Dimethoxymethyl)cyclopentanone	158	C8H14O3	1000424-64-6	64
2	Heptane, 1,1-dimethoxy-	160	C9H20O2	010032-05-0	45
3	Dodecane, 1,1-dimethoxy-	230	C14H30O2	014620-52-1	42
4	2-Propanol, 1,1-dimethoxy-, acetate	162	C7H14O4	074495-37-7	40
5	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	40





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

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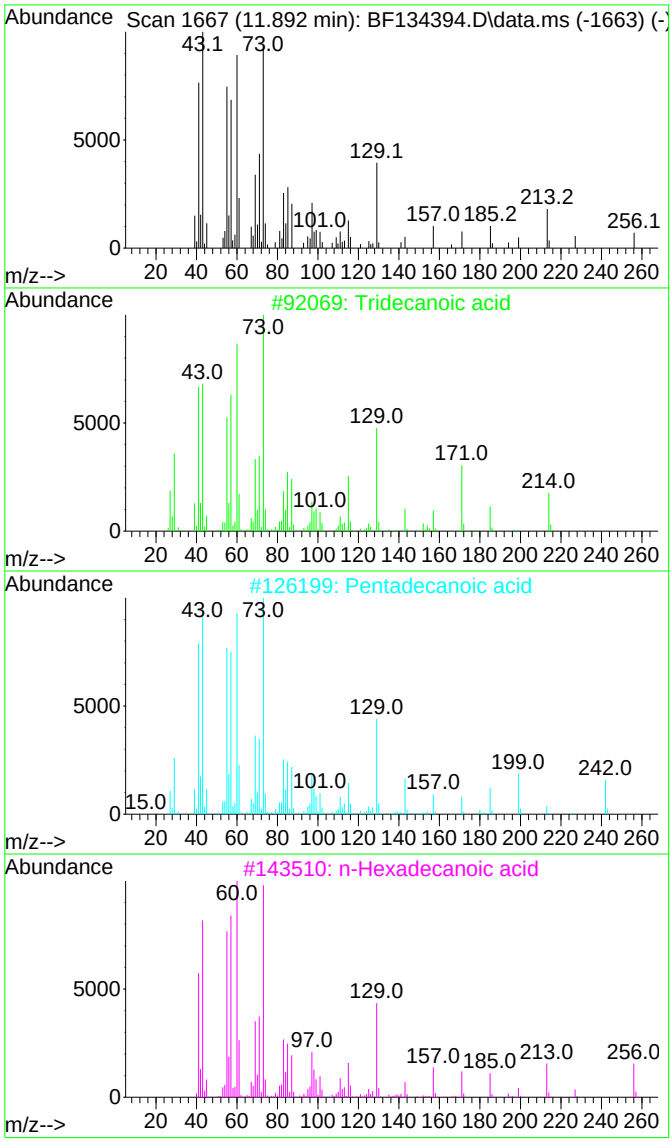
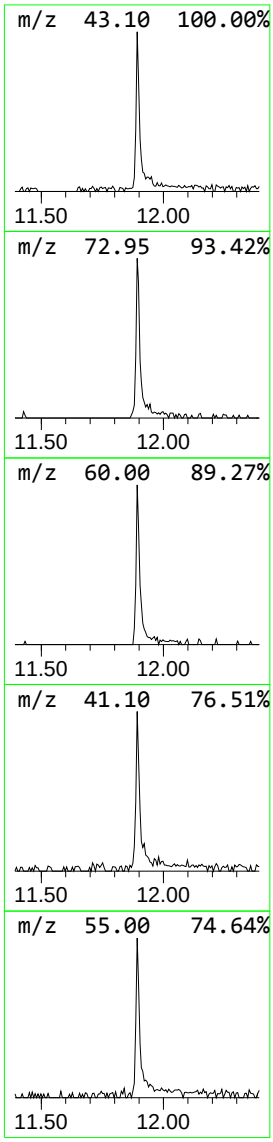
Peak Number 8 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	4.11 ng	115670	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	35
5	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	27





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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...	2.116	67.3	ng	1234840	1	6.834	366987	20.0
Cyclohexene	2.169	241.8	ng	4436480	1	6.834	366987	20.0
unknown5.616	5.616	7.6	ng	138757	1	6.834	366987	20.0
unknown5.663	5.663	13.3	ng	243684	1	6.834	366987	20.0
2-Cyclohexen-1-one	6.092	7.7	ng	140371	1	6.834	366987	20.0
2-Chlorocyclohe...	6.992	14.0	ng	256899	1	6.834	366987	20.0
2-(Dimethoxymet...	7.969	5.0	ng	118005	2	8.116	469536	20.0
Tridecanoic acid	11.892	4.1	ng	115670	4	11.369	562616	20.0