LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#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_P\Methods\8270E-BP091225.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP025865.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.008	7	12	21	rBV	3118862	4543927	62.86%	10.491%
2	4.196	208	214	224	rVB	239469	417074	5.77%	0.963%
3	5.096	360	367	371	rBV	211792	340986	4.72%	0.787%
4	5.384	409	416	429	rVB	1130604	1975724	27.33%	4.561%
5	5.631	453	458	462	rBV	349004	515164	7.13%	1.189%
6	5.831	488	492	504	rVB2	350601	598737	8.28%	1.382%
7	6.361	575	582	587	rVB4	171117	349128	4.83%	0.806%
8	6.637	616	629	634	rBV	722893	1257298	17.39%	2.903%
9	6.749	641	648	652	rBV	261312	437356	6.05%	1.010%
10	6.855	662	666	671	rVB3	280986	482250	6.67%	1.113%
11	6.955	678	683	695	rVB	592459	1143604	15.82%	2.640%
12	7.125	707	712	720	rVV4	147493	330462	4.57%	0.763%
13	7.208	721	726	740	rVB2	248626	568455	7.86%	1.312%
14	7.361	747	752	762	rVB2	311264	542029	7.50%	1.251%
15	7.743	804	817	823	rBV	842675	1843963	25.51%	4.257%
16	8.013	856	863	876	rBV8	188679	580610	8.03%	1.340%
17	8.396	922	928	934	rVB2	284060	495203	6.85%	1.143%
18	8.813	992	999	1006	rBV3	189448	437429	6.05%	1.010%
19	8.896	1006	1013	1019	rBV	1596923	2957992	40.92%	6.829%
20	9.396	1088	1098	1109	rBV2	421629	1504338	20.81%	3.473%
21	9.602	1128	1133	1138	rVB	473504	725527	10.04%	1.675%
22	9.725	1145	1154	1160	rBV3	500667	1296501	17.94%	2.993%
23	10.078	1210	1214	1221	rVB5	199866	389753	5.39%	0.900%
24	10.390	1260	1267	1272	rBV5	396298	938357	12.98%	2.166%
25	10.519	1280	1289	1298	rBV2	1001719	3161275	43.73%	7.299%
26	10.637	1305	1309	1314	rVB	511546	767895	10.62%	1.773%
27	10.707	1318	1321	1327	rVB	294436	439785	6.08%	1.015%
28	11.060	1376	1381	1388	rBV	573620	1209043	16.73%	2.791%
29	11.131	1389	1393	1398	rVV	554293	963135	13.32%	2.224%
30	11.213	1402	1407	1414	rVB2	981885	1983048	27.43%	4.578%
31	11.425	1439	1443	1450	rBV3	403692	878237	12.15%	2.028%
32	11.490	1451	1454	1458	rBV5	323863	553070	7.65%	1.277%
33	12.796	1674	1676	1683	rVB3	956497	1457599	20.17%	3.365%
34	12.984	1702	1708	1717	rBV	3073404	7228319	100.00%	16.688%

Sum of corrected areas: 43313273

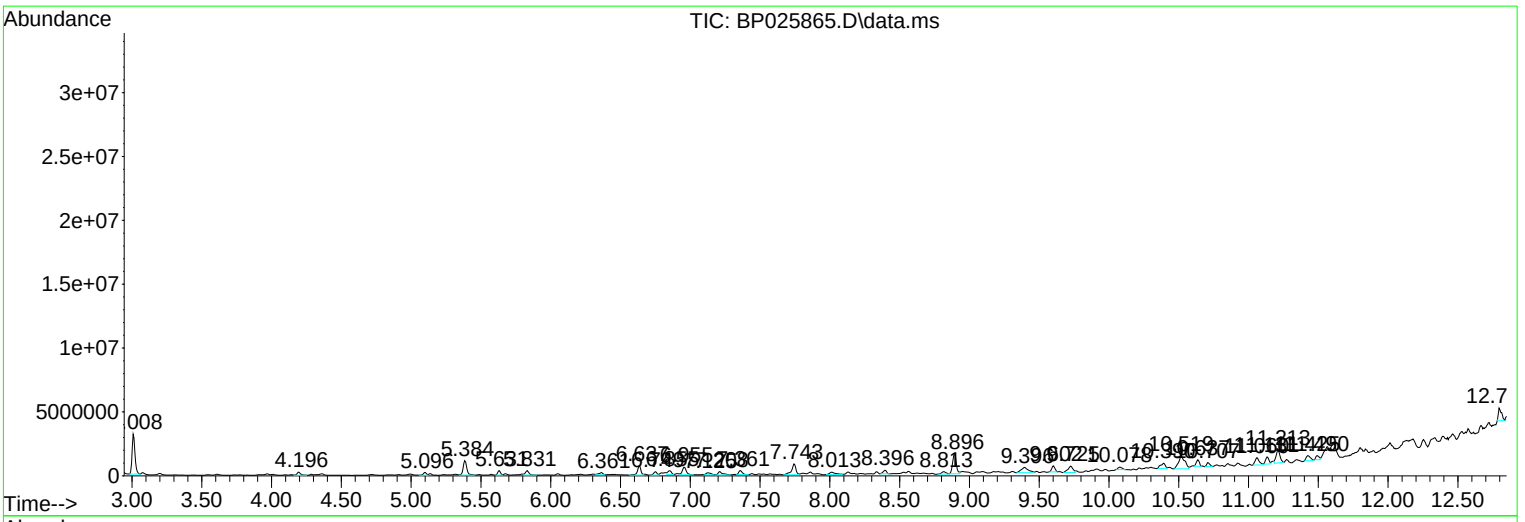
Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

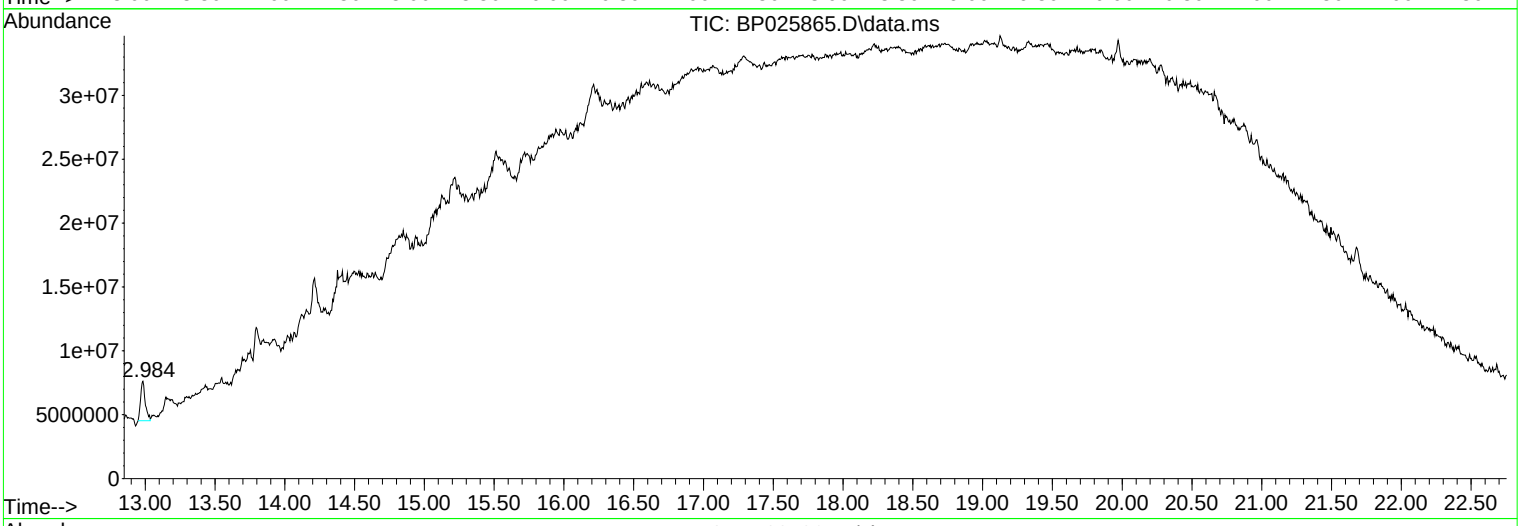
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

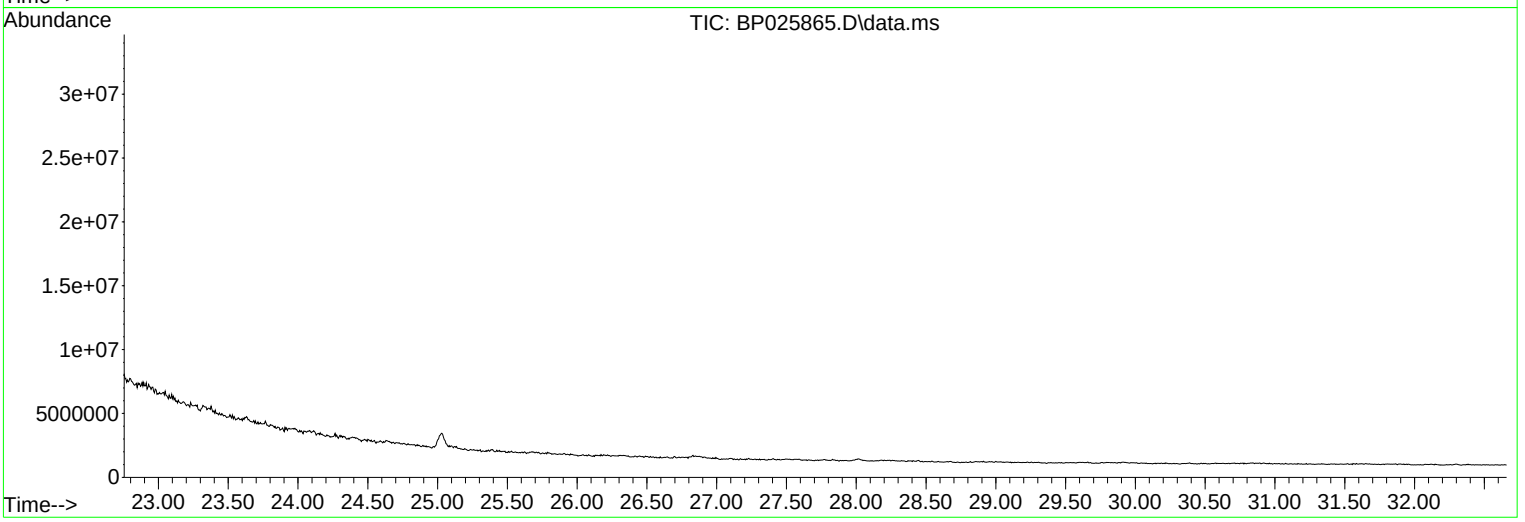
Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

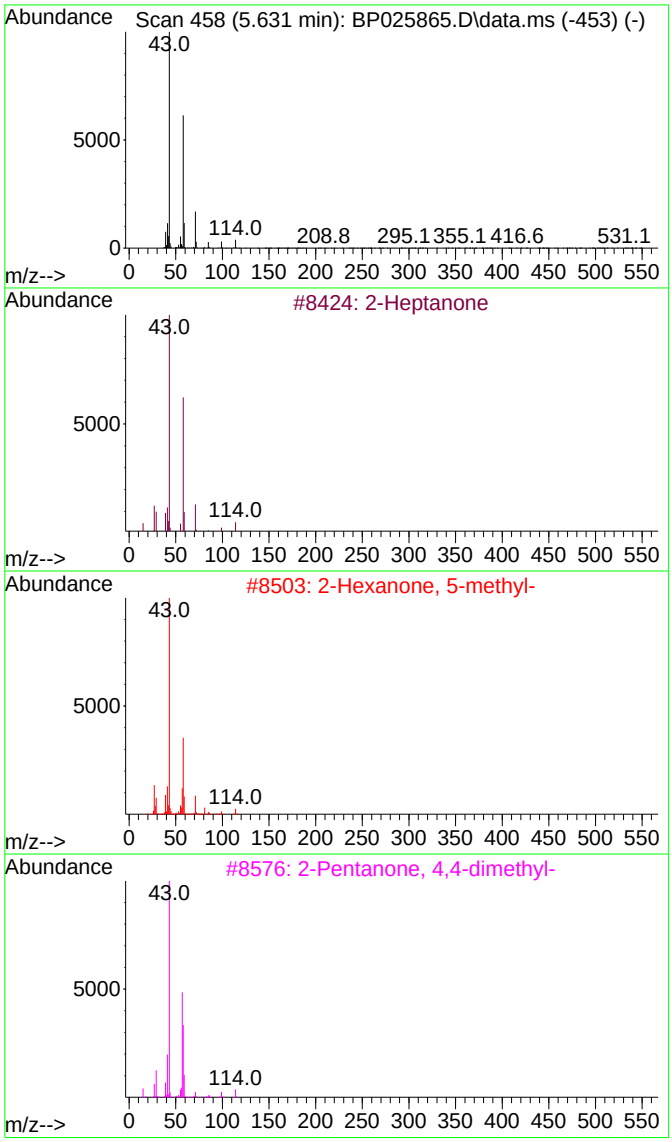
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

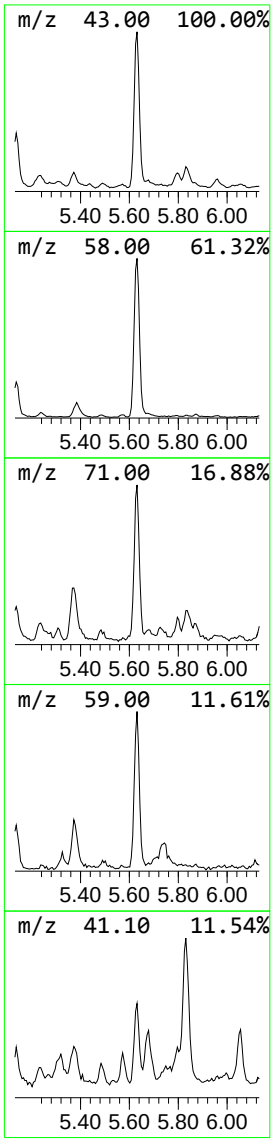
****

Peak Number 2 2-Heptanone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.631	5.59 ng	515164	1,4-Dichlorobenzene-d4	7.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	90
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	90
3	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	50
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	43
5	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

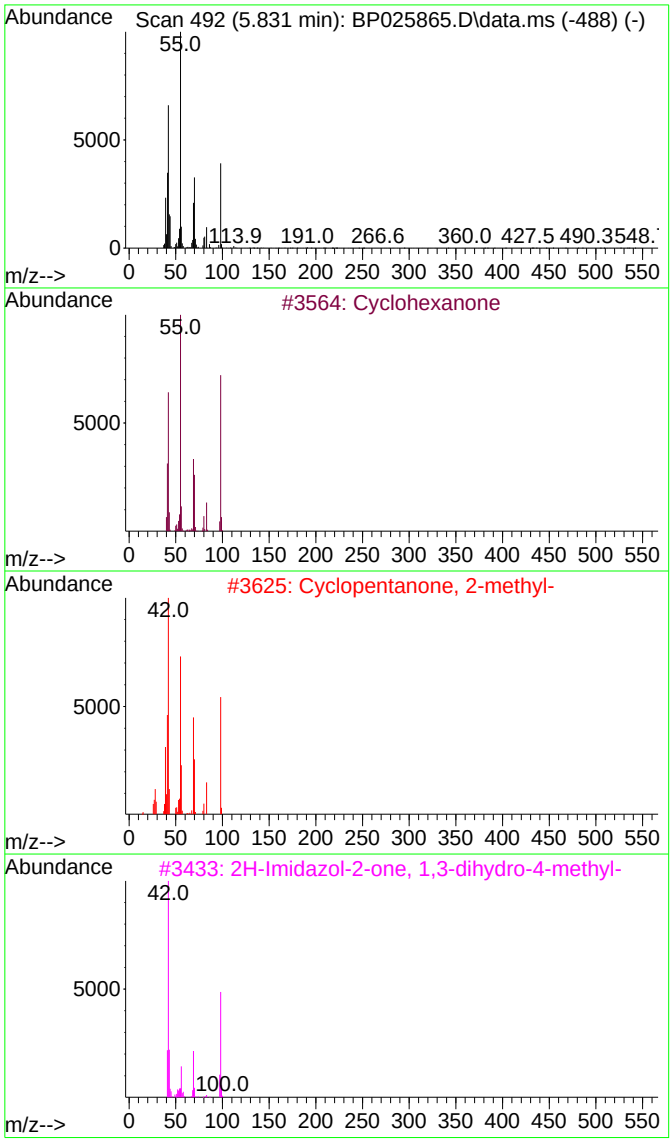
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

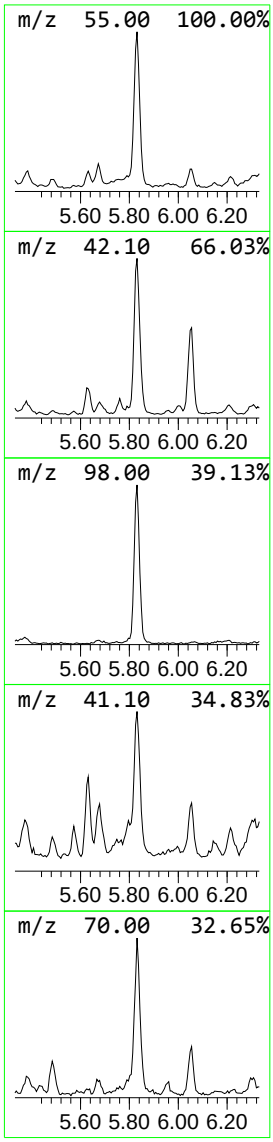
****

Peak Number 3 Cyclohexanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.831	6.49 ng	598737	1,4-Dichlorobenzene-d4	7.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	86
2	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	53
3	2H-Imidazol-2-one, 1,3-dihydro-4...	98	C4H6N2O	001192-34-3	38
4	1-Pentene	70	C5H10	000109-67-1	38
5	3-Penten-2-one, 3-methyl-	98	C6H10O	000565-62-8	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

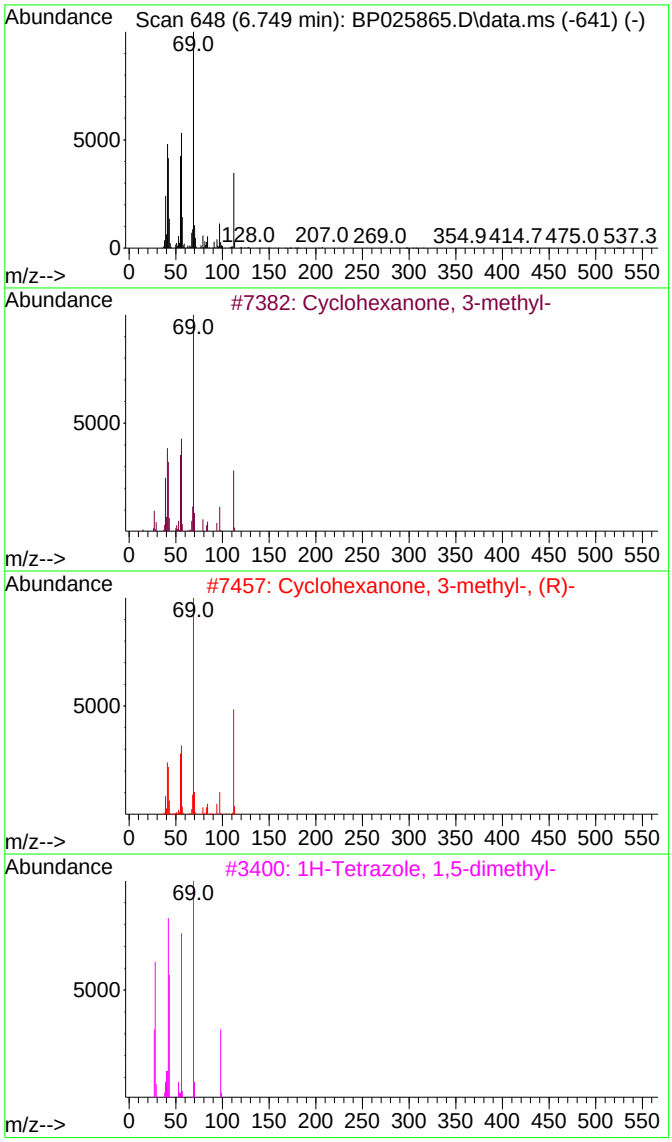
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

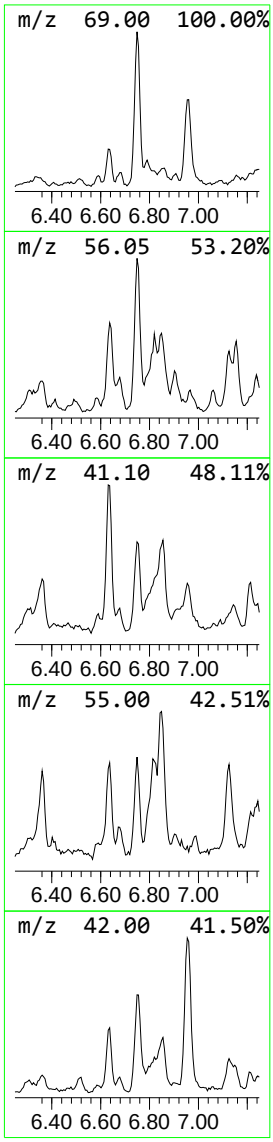
****

Peak Number 5 Cyclohexanone, 3-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.749	4.74 ng	437356	1,4-Dichlorobenzene-d4	7.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3-methyl-	112	C7H12O	000591-24-2	94
2	Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	013368-65-5	91
3	1H-Tetrazole, 1,5-dimethyl-	98	C3H6N4	005144-11-6	59
4	2-Methyl-2-heptene	112	C8H16	000627-97-4	52
5	ICN 3847	324	C8H13N4O8P	040925-28-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

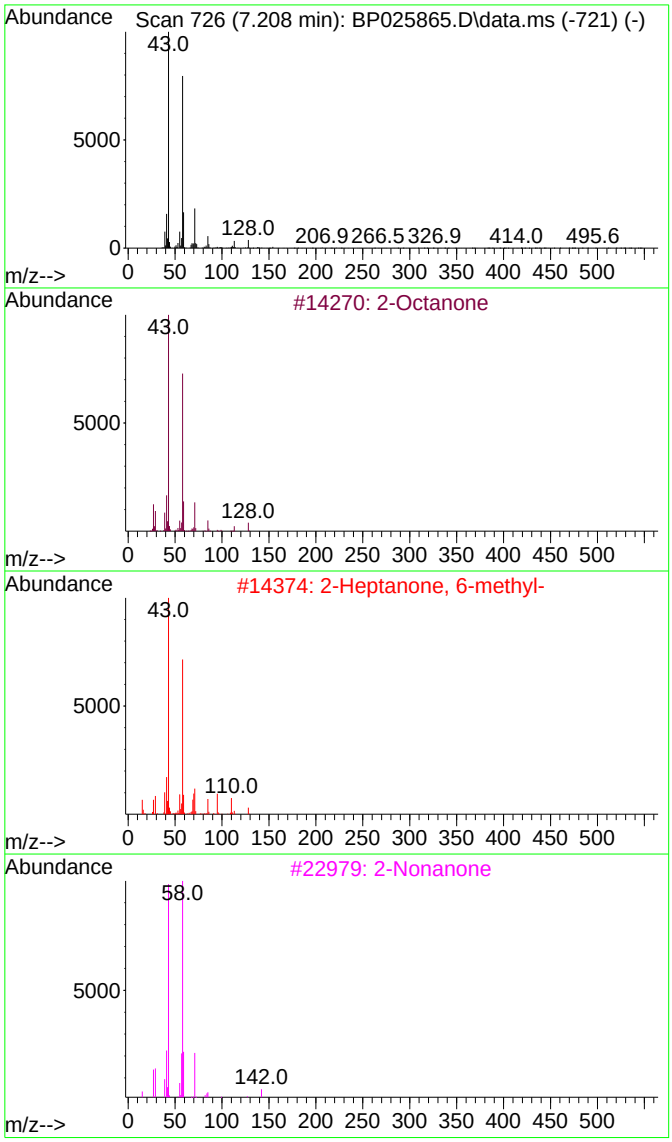
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

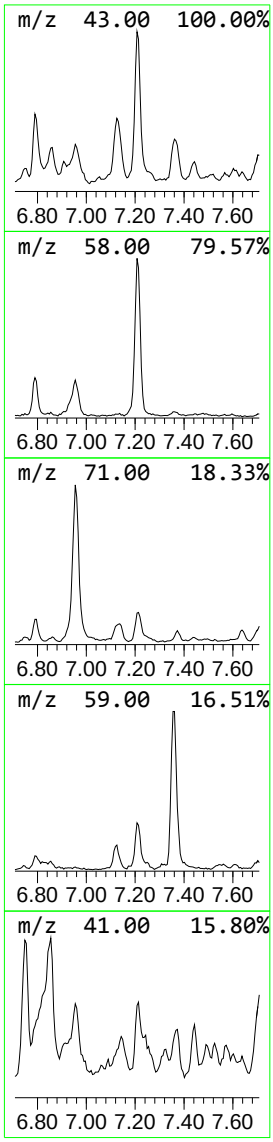
****

Peak Number 7 2-Octanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	6.17 ng	568455	1,4-Dichlorobenzene-d4	7.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	94
2	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	78
3	2-Nonanone	142	C9H18O	000821-55-6	78
4	2-Heptanone	114	C7H14O	000110-43-0	72
5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

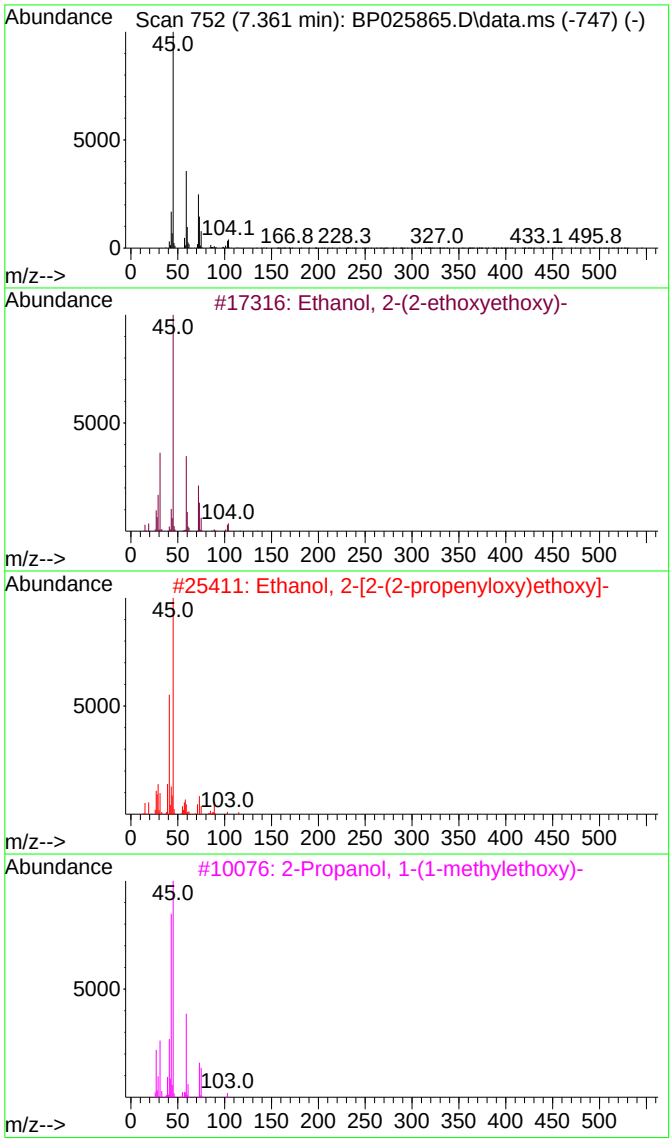
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

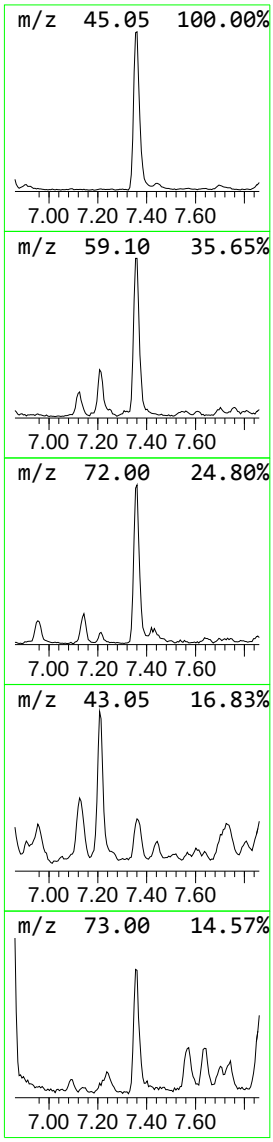
****

Peak Number 8 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.361	5.88 ng	542029	1,4-Dichlorobenzene-d4	7.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	47
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Methoxymethyl isothiocyanate	103	C3H5NOS	019900-84-6	42
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

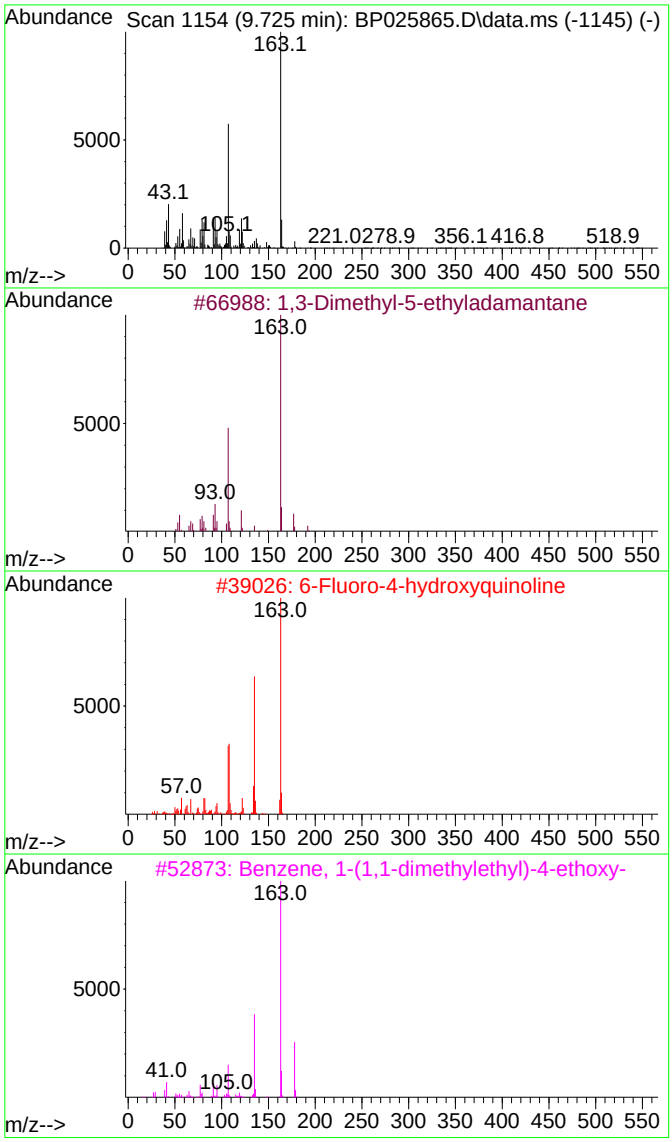
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

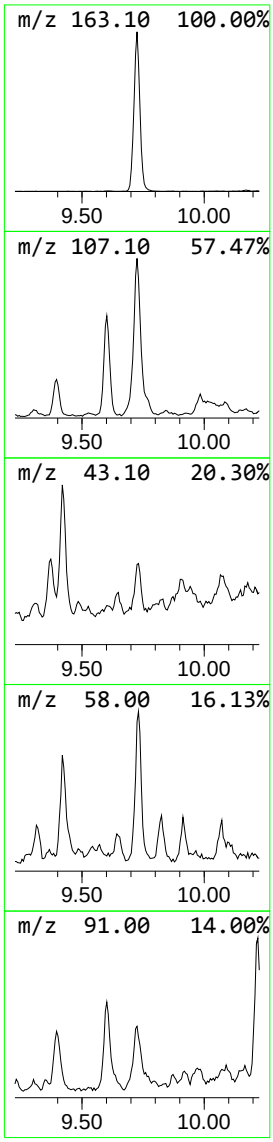
****

Peak Number 14 1,3-Dimethyl-5-ethyladamantane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.725	8.20 ng	1296500	Naphthalene-d8	10.519

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	86
2	6-Fluoro-4-hydroxyquinoline	163	C9H6FNO	000391-78-6	53
3	Benzene, 1-(1,1-dimethylethyl)-4...	178	C12H18O	017269-94-2	50
4	6-Amino-2,4-dimethyl-5,7-diazabe...	163	C8H9N3O	022727-43-1	50
5	2,3-Benzofurandione 2-monooxime	163	C8H5NO3	040701-27-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

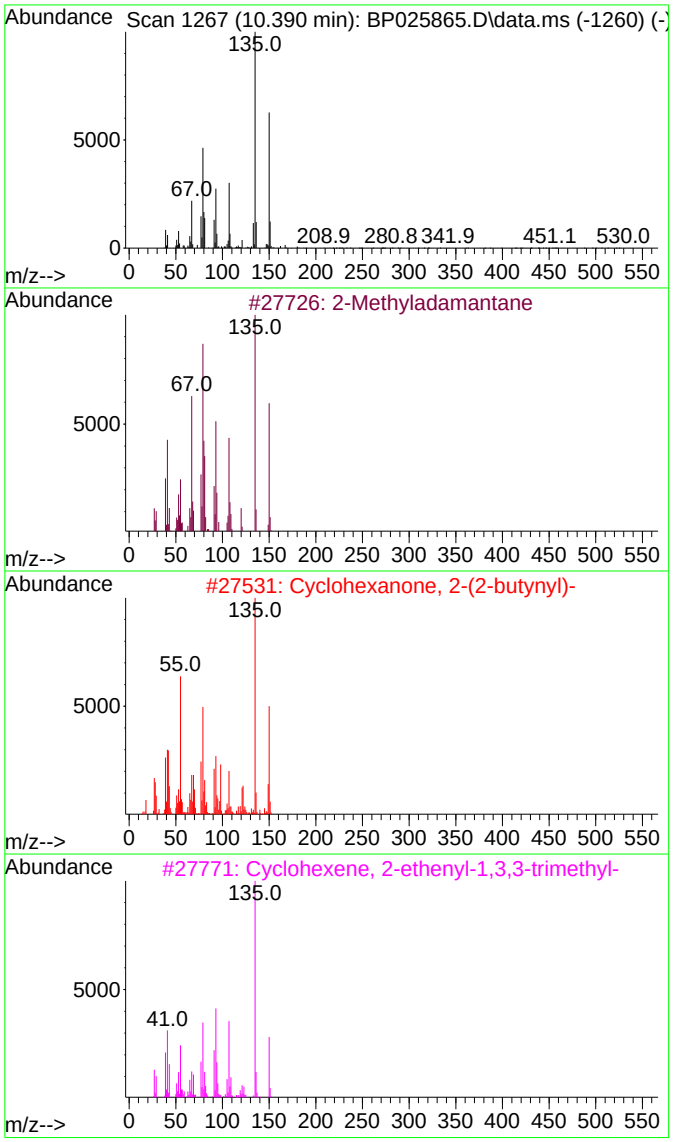
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

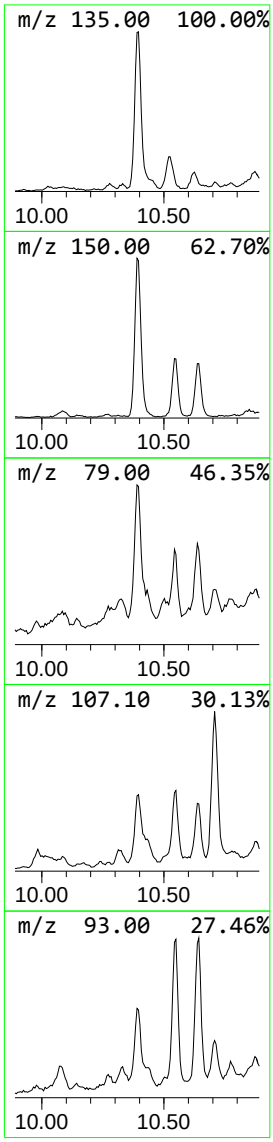
****

Peak Number 15 2-Methyladamantane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.390	5.94 ng	938357	Naphthalene-d8	10.519

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyladamantane	150	C11H18	000700-56-1	86
2	Cyclohexanone, 2-(2-butynyl)-	150	C10H14O	054166-48-2	80
3	Cyclohexene, 2-ethenyl-1,3,3-tri...	150	C11H18	005293-90-3	72
4	Y-Methylbicyclo(4.3.0)non-6-en-8...	150	C10H14O	1000424-65-9	62
5	1-Adamantyl methyl ketone	178	C12H18O	001660-04-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

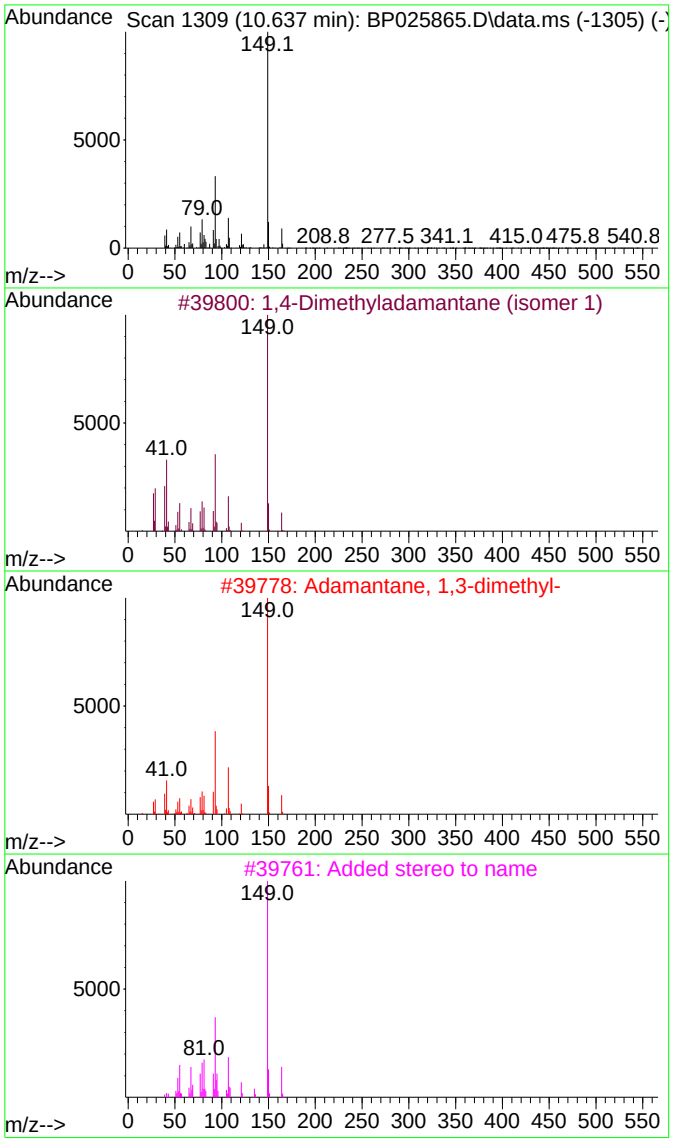
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

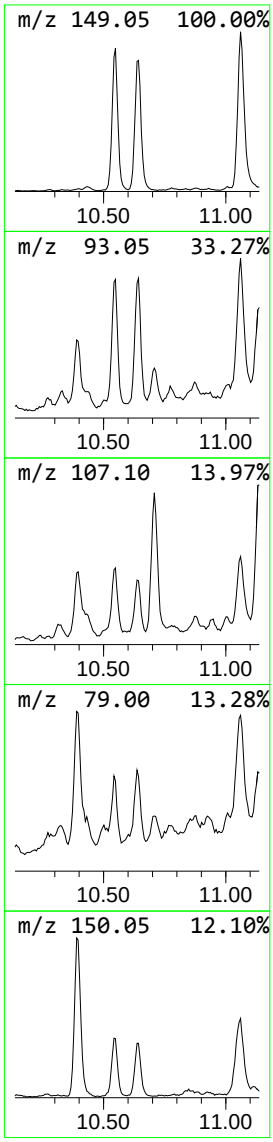
****

Peak Number 16 1,4-Dimethyladamantane (iso... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.637	4.86 ng	767895	Naphthalene-d8	10.519

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	91
2	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	87
3	Added stereo to name	164	C12H20	024145-89-9	83
4	2-(3-Methylbuta-1,3-dienyl)cyclo...	164	C11H16O	1000191-75-5	64
5	1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

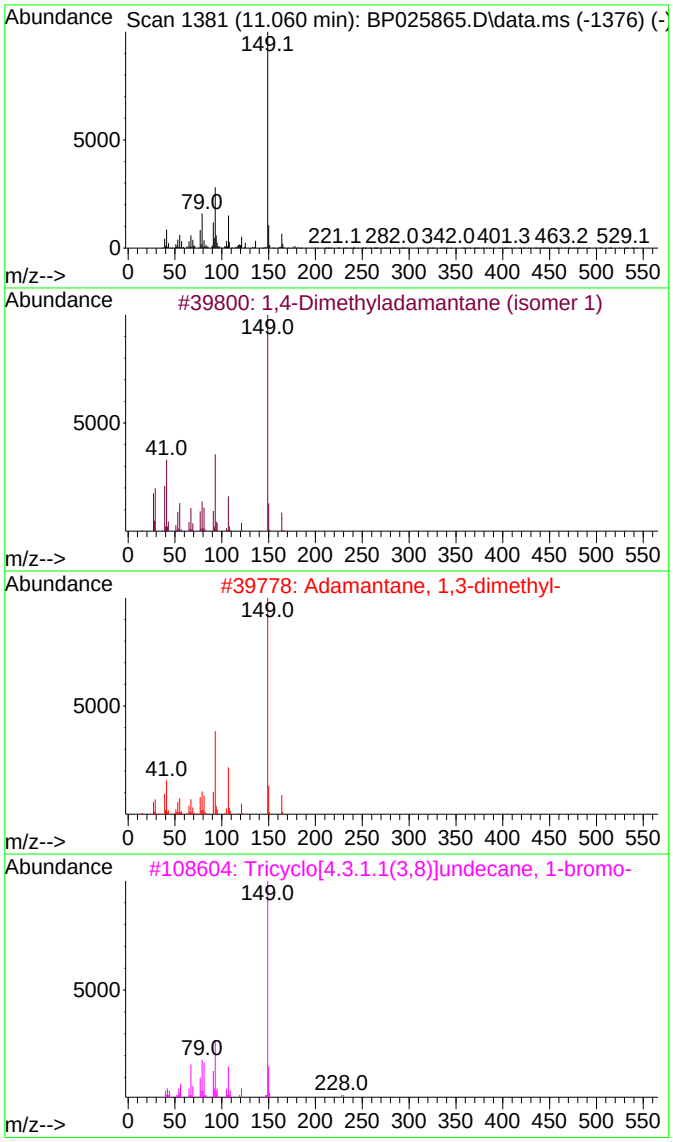
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

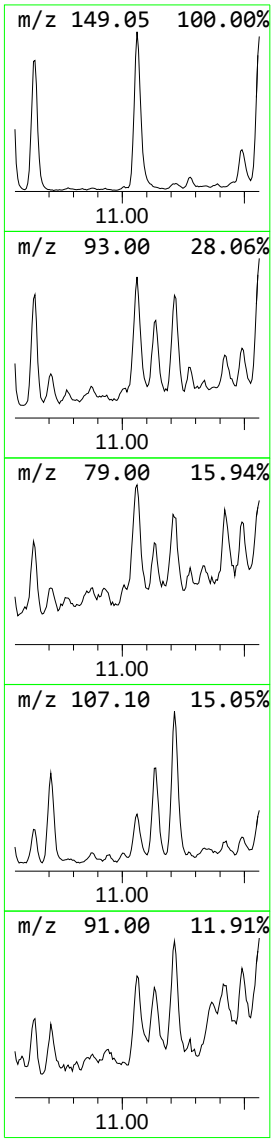
****

Peak Number 17 Adamantane, 1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.060	7.65 ng	1209040	Naphthalene-d8	10.519

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	91
2	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	90
3	Tricyclo[4.3.1.1(3,8)]undecane, ...	228	C11H17Br	021898-96-4	74
4	Tricyclo[4.3.1.1(3,8)]undecane, ...	184	C11H17Cl	027011-46-7	64
5	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092525\
Data File : BP025865.D
Acq On : 25 Sep 2025 20:13
Operator : CG/JU
Sample : Q3168-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TOTES COMP#2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091225.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
2-Heptanone	5.631	5.6	ng	515164	1	7.749	1843960	20.0
Cyclohexanone	5.831	6.5	ng	598737	1	7.749	1843960	20.0
Cyclohexanone, ...	6.749	4.7	ng	437356	1	7.749	1843960	20.0
2-Octanone	7.208	6.2	ng	568455	1	7.749	1843960	20.0
Ethanol, 2-(2-e...	7.361	5.9	ng	542029	1	7.749	1843960	20.0
1,3-Dimethyl-5-...	9.725	8.2	ng	1296500	2	10.519	3161280	20.0
2-Methyladamantane	10.390	5.9	ng	938357	2	10.519	3161280	20.0
1,4-Dimethylada...	10.637	4.9	ng	767895	2	10.519	3161280	20.0
Adamantane, 1,3...	11.060	7.7	ng	1209040	2	10.519	3161280	20.0