

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081925\
 Data File : BP025483.D
 Acq On : 19 Aug 2025 19:39
 Operator : CG/JU
 Sample : Q2815-13
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TW-22M-E

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-BP081425.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP025483.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.043	13	18	35	rVB	2836460	3863262	22.50%	7.498%
2	4.966	335	345	350	rBV	8699134	17173715	100.00%	33.330%
3	5.408	414	420	432	rBV	455322	698771	4.07%	1.356%
4	6.966	678	685	699	rBV	143329	269210	1.57%	0.522%
5	7.790	818	825	832	rBV	680573	1102416	6.42%	2.140%
6	8.931	1011	1019	1027	rBV	715121	1272918	7.41%	2.470%
7	10.560	1288	1296	1305	rBV	885031	1522318	8.86%	2.954%
8	13.013	1705	1713	1724	rBV	1806953	2801974	16.32%	5.438%
9	14.407	1938	1950	1962	rBV	1265129	2065216	12.03%	4.008%
10	15.601	2145	2153	2158	rBV	354237	512013	2.98%	0.994%
11	15.654	2158	2162	2174	rVB	594575	818289	4.76%	1.588%
12	15.778	2177	2183	2192	rBV	1136157	1801500	10.49%	3.496%
13	15.913	2199	2206	2215	rBV	651600	1087534	6.33%	2.111%
14	16.036	2222	2227	2235	rVB2	143249	210459	1.23%	0.408%
15	16.354	2270	2281	2291	rVB	176336	273692	1.59%	0.531%
16	17.207	2418	2426	2433	rBV2	1525592	2506739	14.60%	4.865%
17	19.630	2833	2838	2844	rBV	177543	230301	1.34%	0.447%
18	19.919	2881	2887	2894	rBV	3142147	4701694	27.38%	9.125%
19	21.019	3070	3074	3083	rVB	540158	731760	4.26%	1.420%
20	21.313	3120	3124	3137	rBV2	849417	1480483	8.62%	2.873%
21	21.642	3175	3180	3195	rVB2	1858384	2882373	16.78%	5.594%
22	21.907	3222	3225	3232	rVB	126897	192401	1.12%	0.373%
23	22.566	3333	3337	3346	rVB4	129117	267928	1.56%	0.520%
24	25.024	3745	3755	3767	rVB2	1091954	3059646	17.82%	5.938%

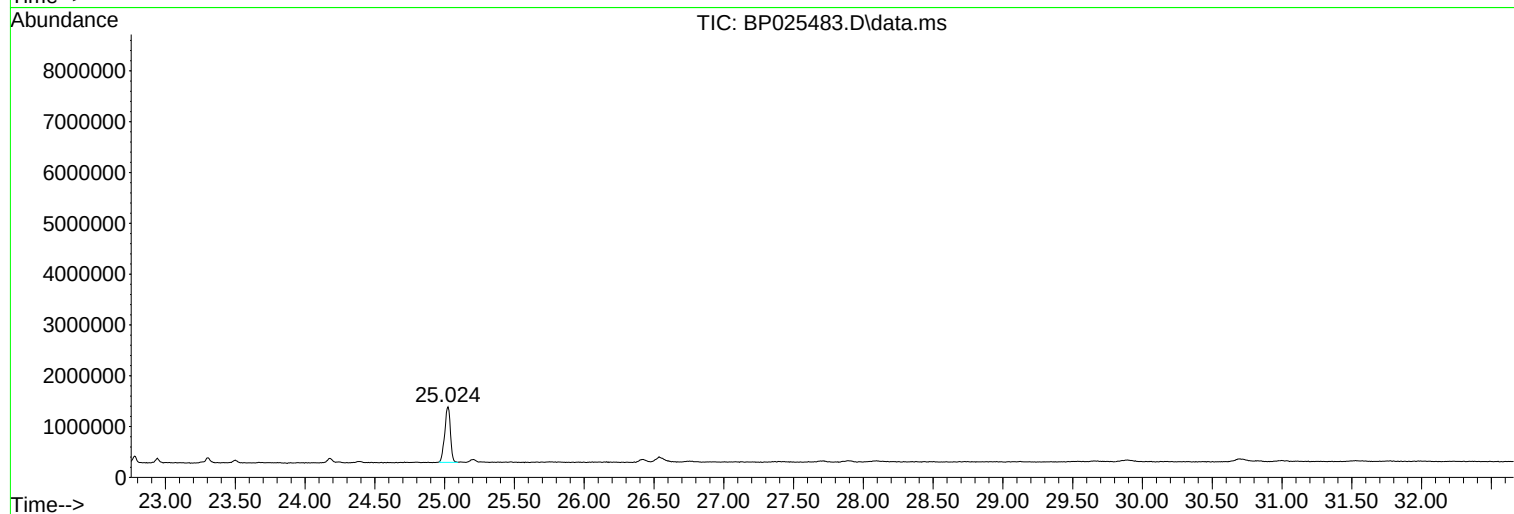
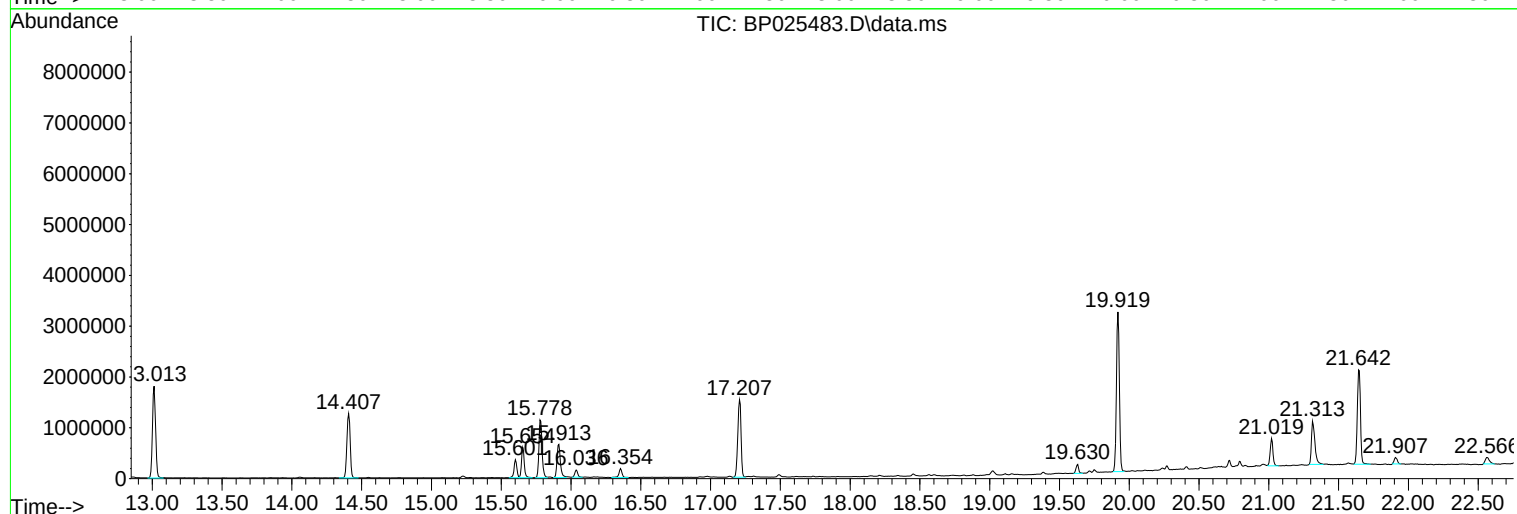
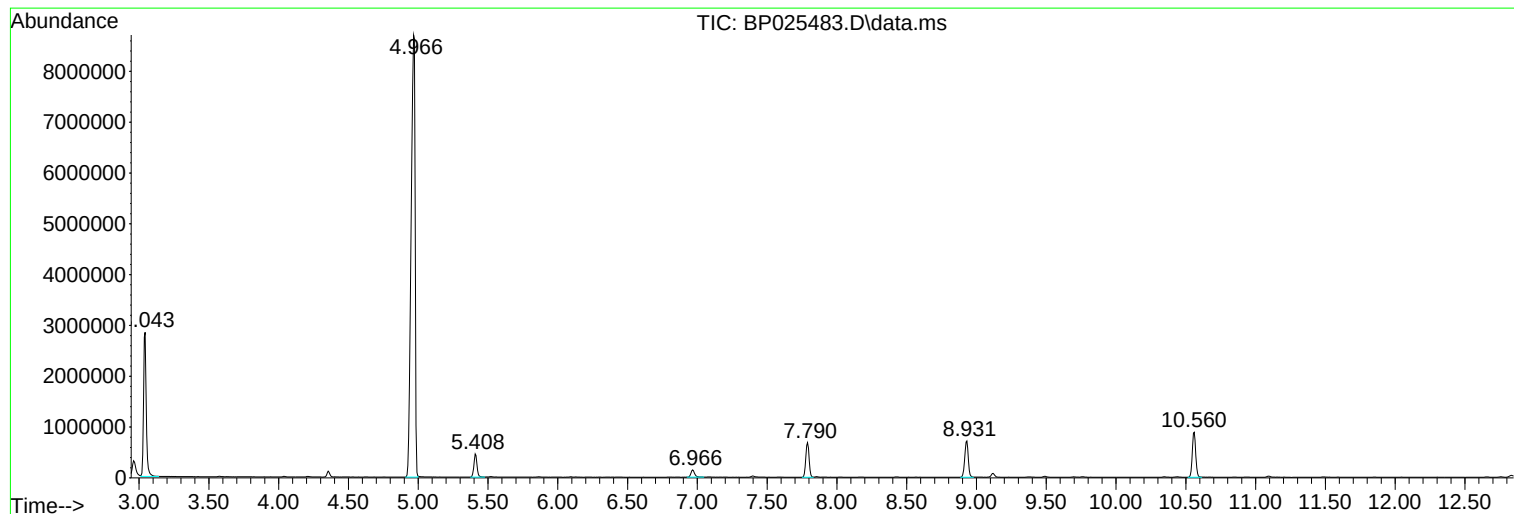
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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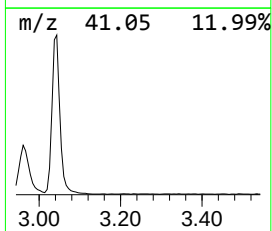
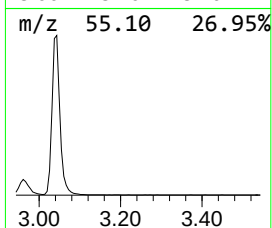
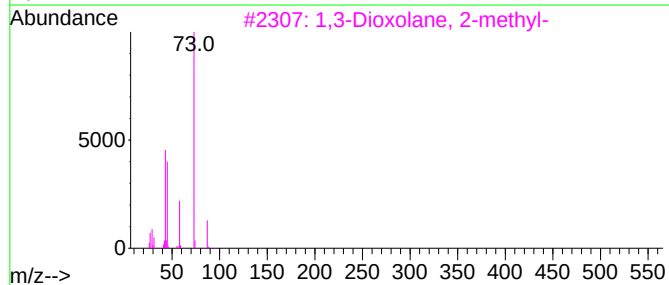
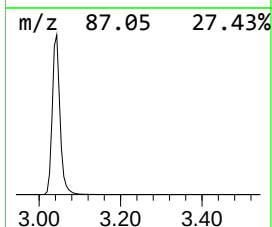
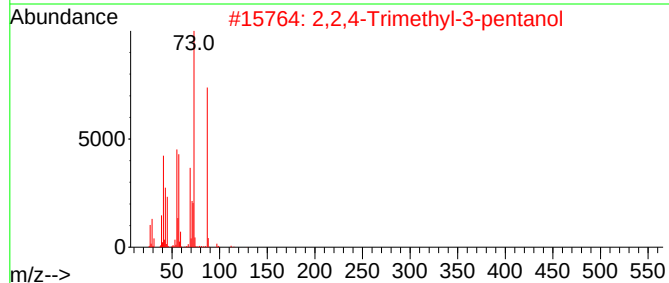
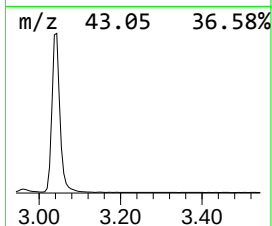
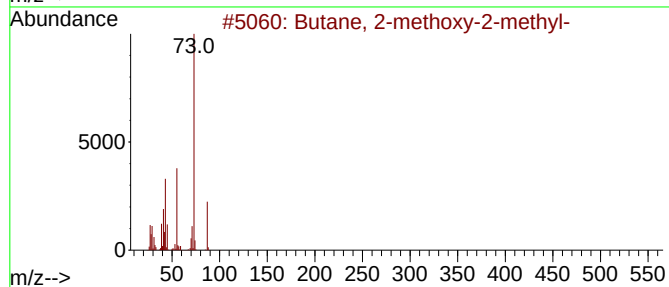
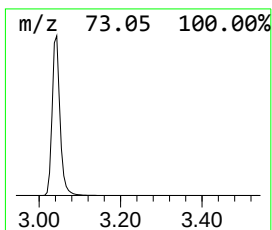
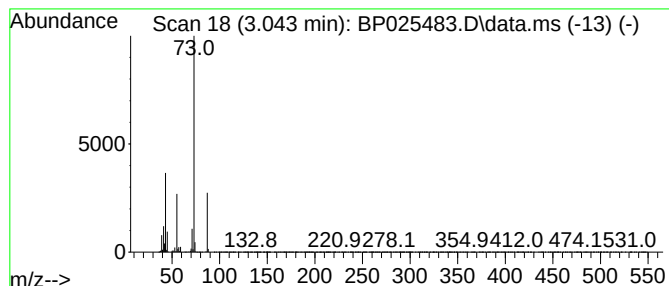
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.043	70.09 ng	3863260	1,4-Dichlorobenzene-d4	7.790

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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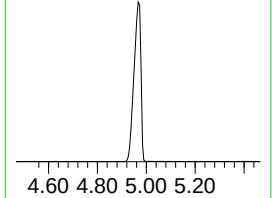
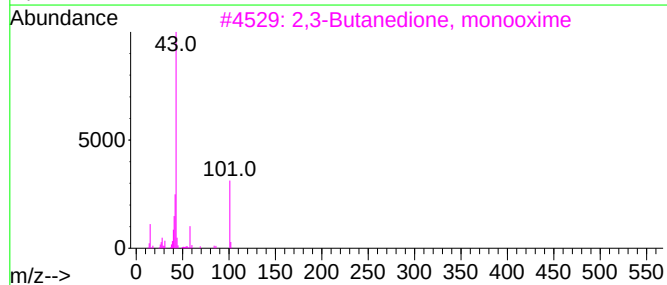
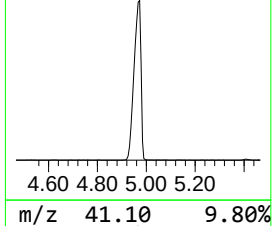
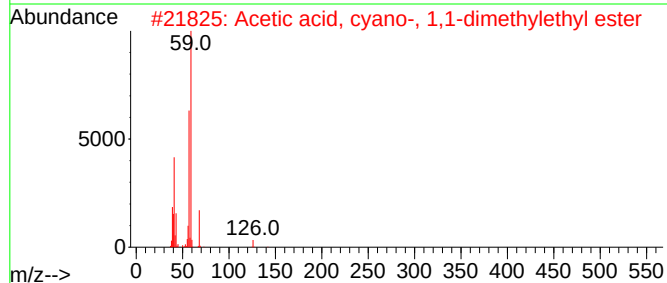
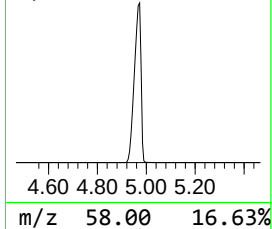
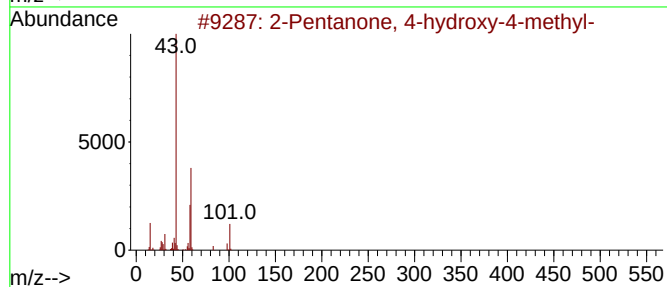
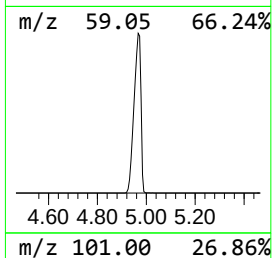
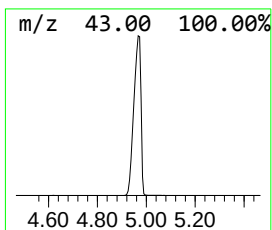
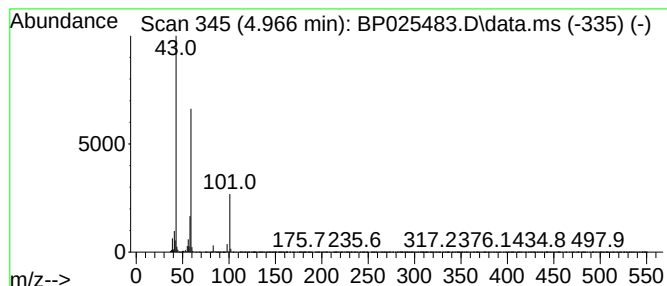
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.966	311.57 ng	17173700	1,4-Dichlorobenzene-d4	7.790

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Acetone	58	C3H6O	000067-64-1	10
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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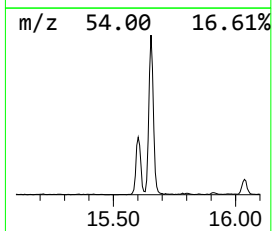
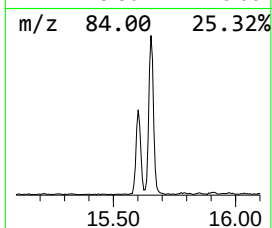
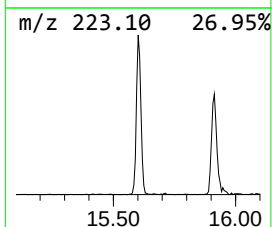
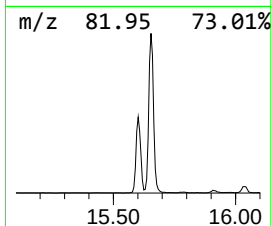
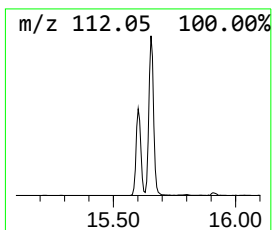
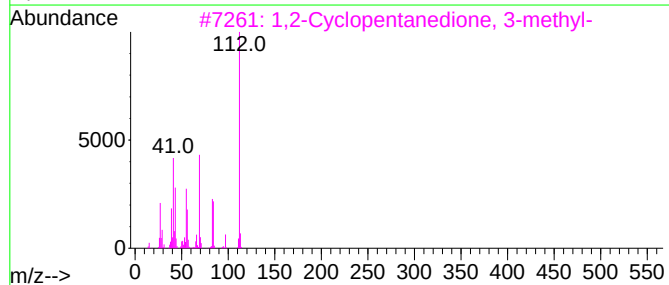
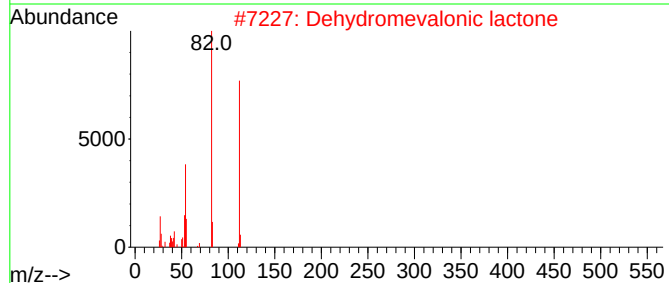
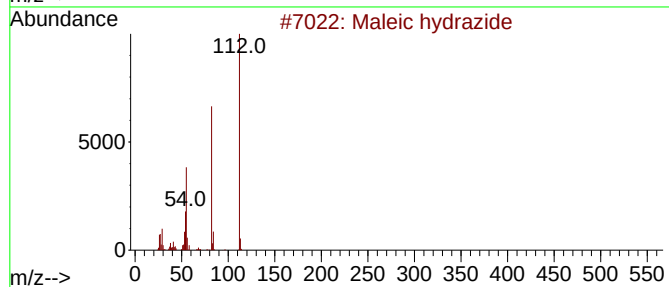
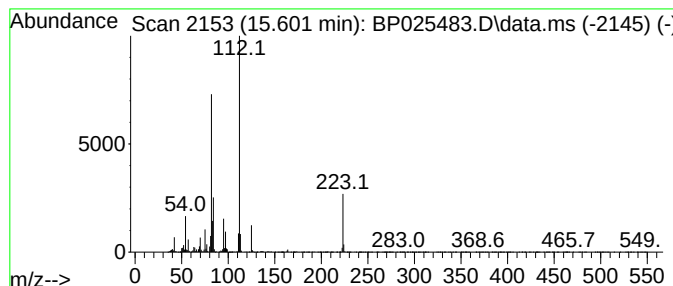
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Maleic hydrazide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.601	4.96 ng	512013	Acenaphthene-d10	14.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Maleic hydrazide	112	C4H4N2O2	000123-33-1	50
2			Dehydromevalonic lactone	112	C6H8O2	002381-87-5	47
3			1,2-Cyclopentanedione, 3-methyl-	112	C6H8O2	000765-70-8	46
4			4H-1,2,4-Triazol-3-amine, 4-ethyl-	112	C4H8N4	042786-06-1	43
5			2-Hydroxy-5-ethyl-5-methylcyclop...	140	C8H12O2	053263-57-3	38



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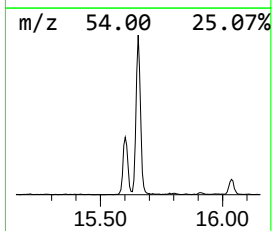
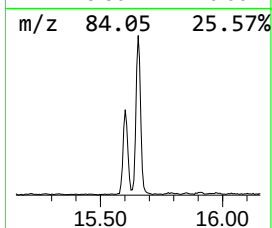
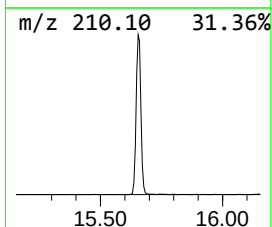
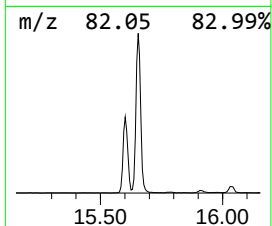
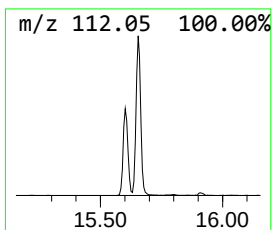
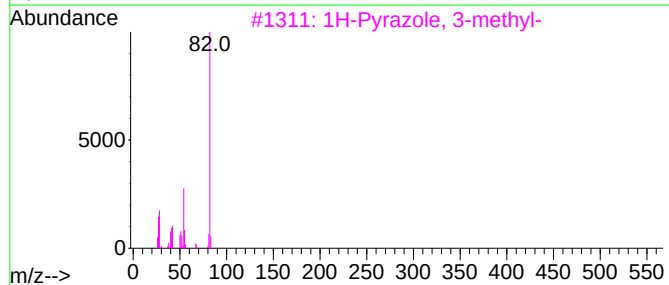
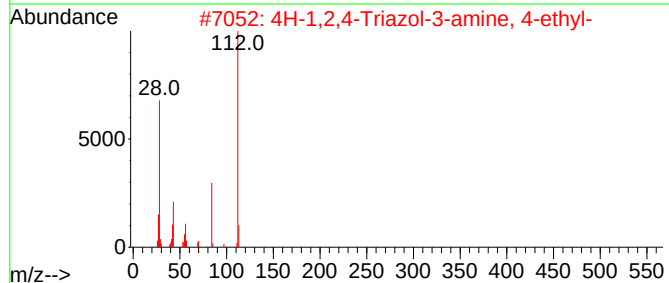
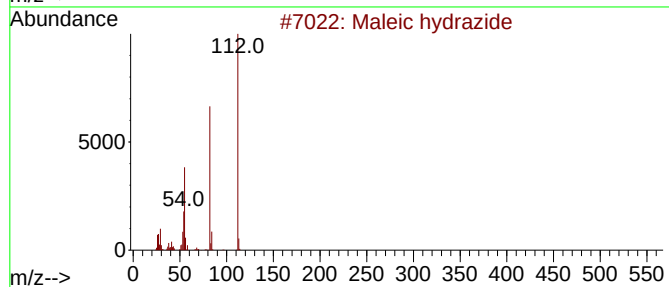
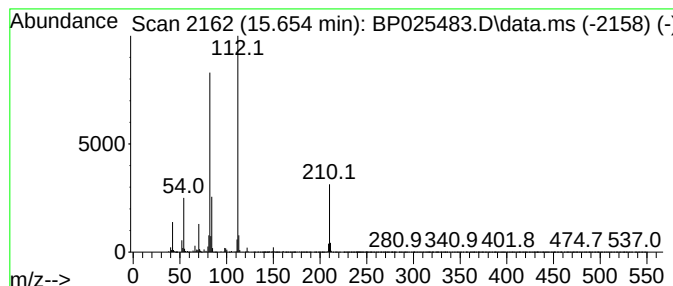
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.92 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.654	7.92 ng	818289	Acenaphthene-d10	14.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Maleic hydrazide	112	C4H4N2O2	000123-33-1	59
2			4H-1,2,4-Triazol-3-amine, 4-ethyl-	112	C4H8N4	042786-06-1	35
3			1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	30
4			1H-Imidazole, 1-methyl-	82	C4H6N2	000616-47-7	27
5			3H-Pyrazol-3-one, 2,4-dihydro-2,...	112	C5H8N2O	002749-59-9	27



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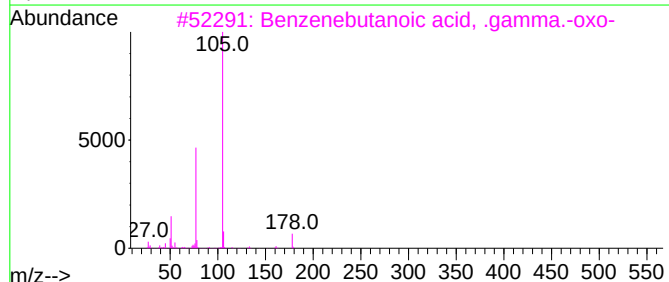
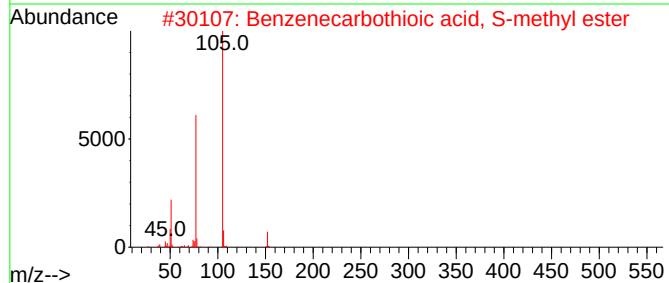
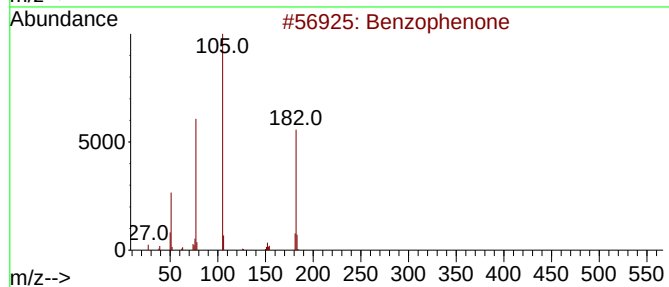
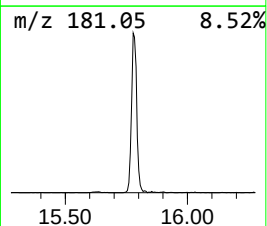
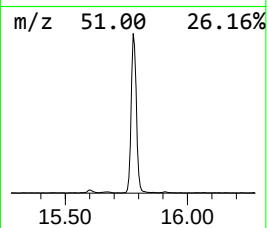
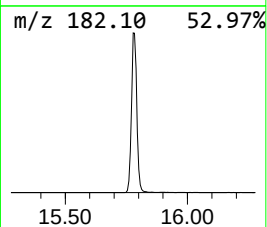
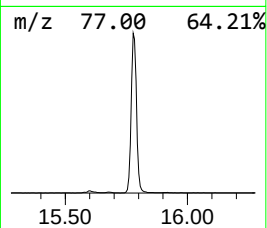
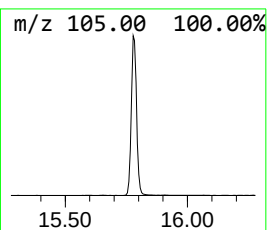
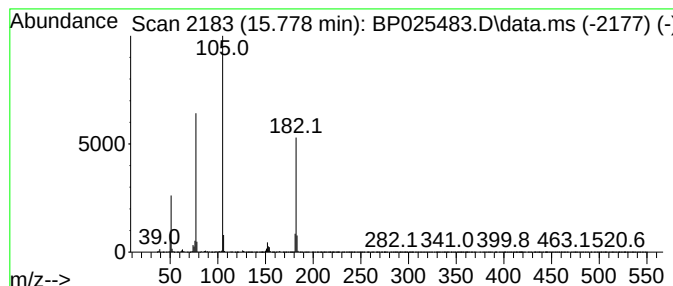
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.778	17.45 ng	1801500	Acenaphthene-d10	14.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	49
4			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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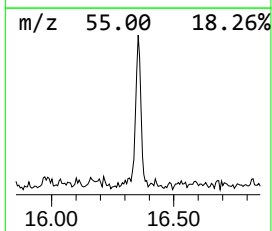
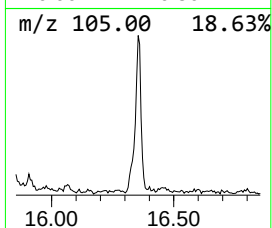
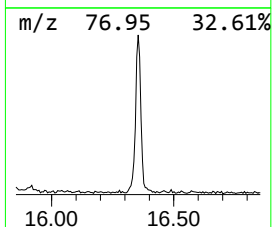
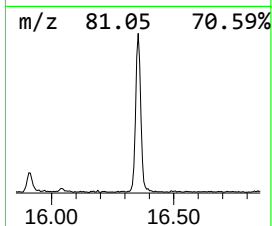
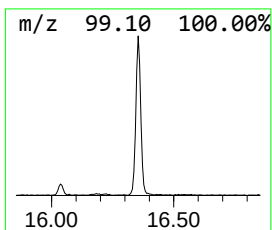
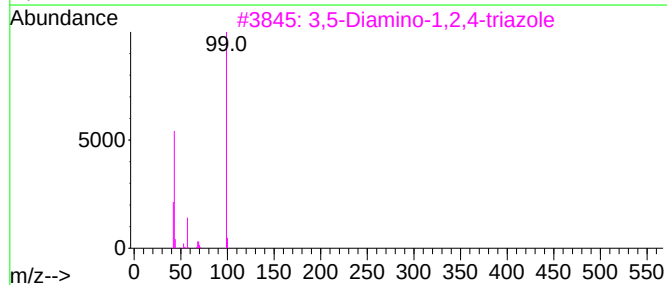
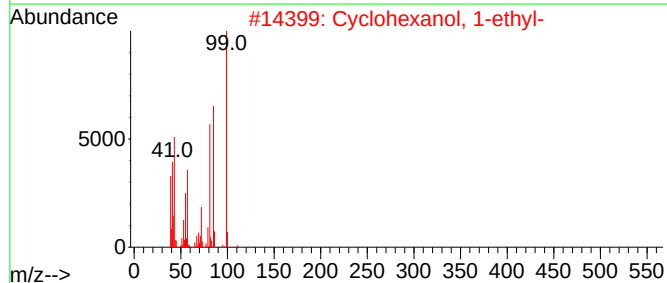
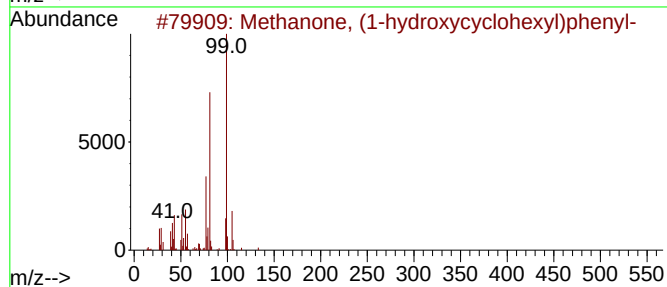
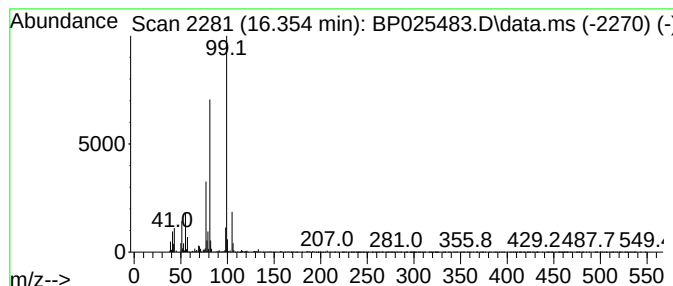
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methanone, (1-hydroxycyclohexyl) Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.354	2.18 ng	273692	Phenanthrene-d10	17.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2			Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	50
3			3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	43
4			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	40
5			Hexanoic acid, thio-, S-butyl ester	188	C10H20O5	002432-79-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081925\
Data File : BP025483.D
Acq On : 19 Aug 2025 19:39
Operator : CG/JU
Sample : Q2815-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

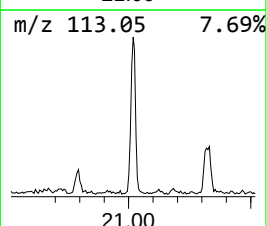
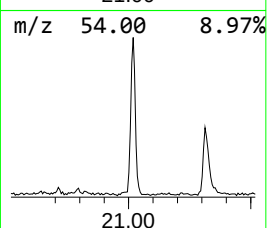
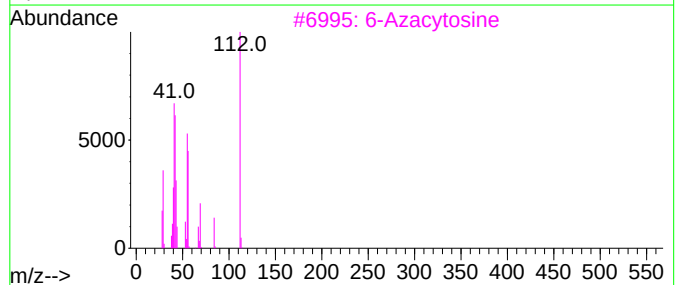
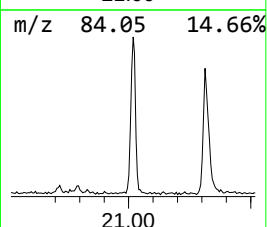
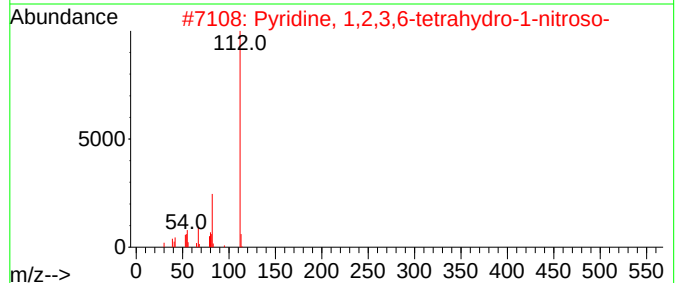
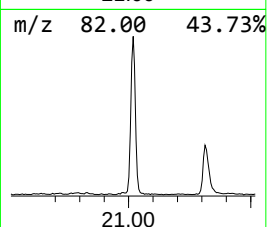
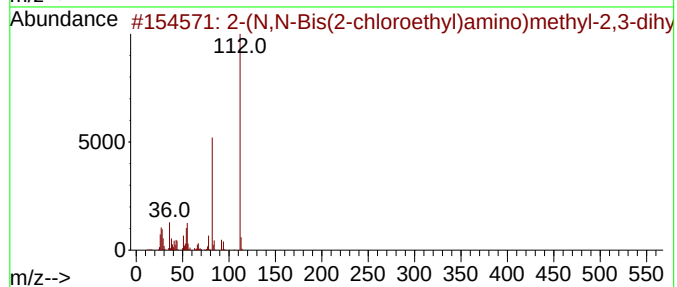
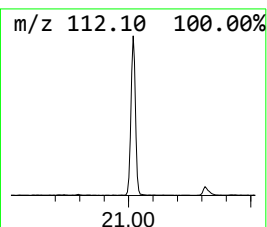
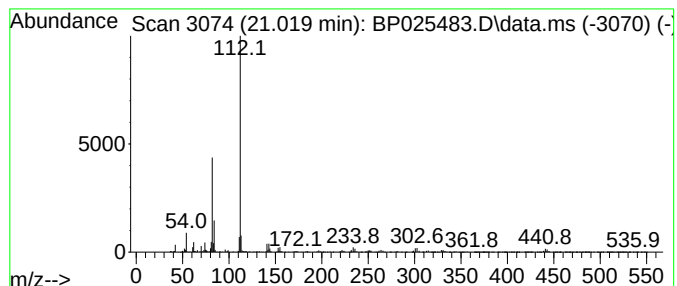
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ClientSampleId :
TW-22M-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.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-(N,N-Bis(2-chloroethyl)am... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.019	5.08 ng	731760	Chrysene-d12	21.642	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(N,N-Bis(2-chloroethyl)amino)m...	265	C9H13Cl12N3O2	014628-36-5	56
2	Pyridine, 1,2,3,6-tetrahydro-1-n...	112	C5H8N2O	055556-92-8	50
3	6-Azacytosine	112	C3H4N4O	000931-85-1	47
4	Sulfide,1- propenyl 1-propynyl	112	C6H8S	089533-93-7	43
5	2-Cyclopenten-1-one, 2-hydroxy-3...	112	C6H8O2	000080-71-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081925\
Data File : BP025483.D
Acq On : 19 Aug 2025 19:39
Operator : CG/JU
Sample : Q2815-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TW-22M-E

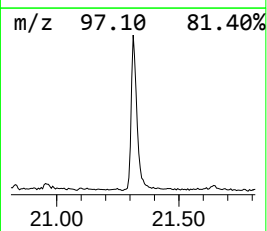
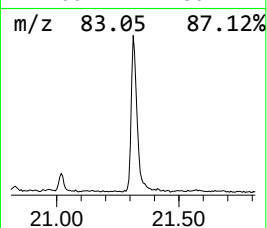
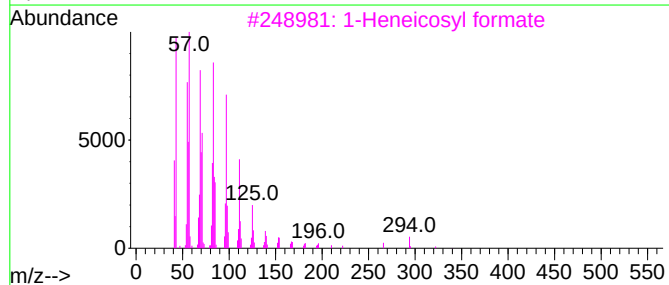
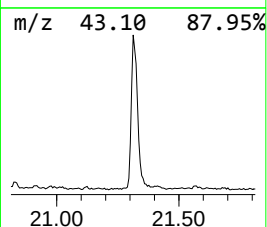
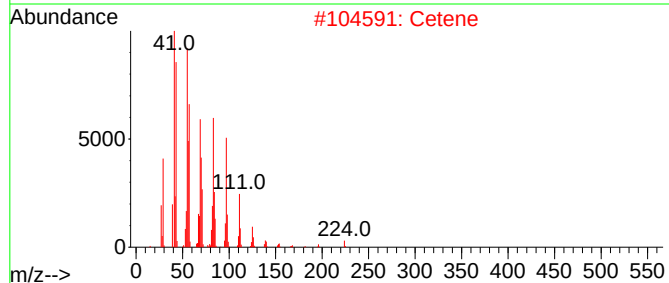
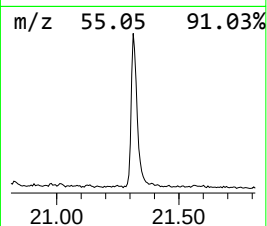
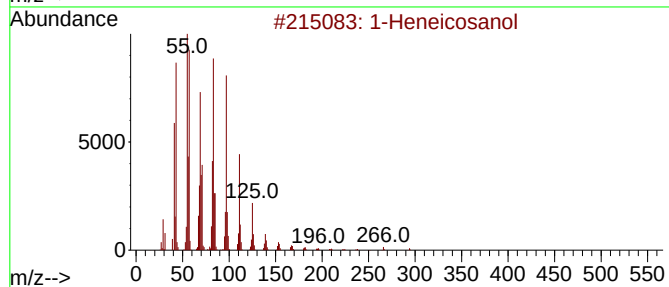
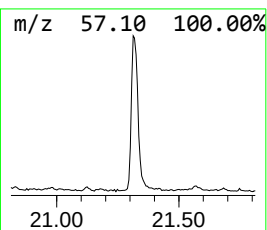
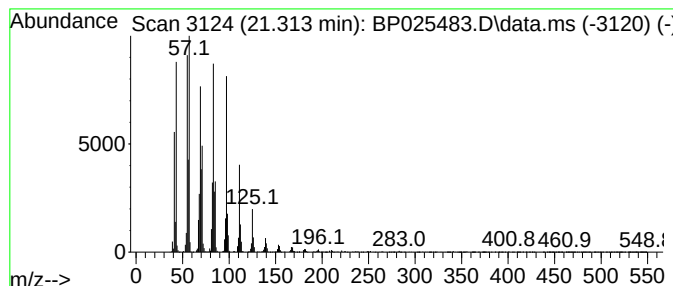
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.313	10.27 ng	1480480	Chrysene-d12	21.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Cetene	224	C16H32	000629-73-2	95
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081925\
Data File : BP025483.D
Acq On : 19 Aug 2025 19:39
Operator : CG/JU
Sample : Q2815-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TW-22M-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.043	70.1	ng	3863260	1	7.790	1102420	20.0
2-Pentanone, 4-...	4.966	311.6	ng	17173700	1	7.790	1102420	20.0
Maleic hydrazide	15.601	5.0	ng	512013	3	14.407	2065220	20.0
unknown7.92	15.654	7.9	ng	818289	3	14.407	2065220	20.0
Benzophenone	15.778	17.4	ng	1801500	3	14.407	2065220	20.0
Methanone, (1-h...	16.354	2.2	ng	273692	4	17.207	2506740	20.0
2-(N,N-Bis(2-ch...	21.019	5.1	ng	731760	5	21.642	2882370	20.0
1-Heneicosanol	21.313	10.3	ng	1480480	5	21.642	2882370	20.0