

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
 Data File : BF143717.D
 Acq On : 11 Sep 2025 20:27
 Operator : RC/JU
 Sample : Q3075-06
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MOO-25-0259

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-BF091025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143717.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.193	334	340	349	rBV	51401	78402	1.56%	0.711%
2	5.110	487	496	502	rBB	65315	99549	1.98%	0.903%
3	5.504	557	563	568	rBV	456454	594338	11.84%	5.393%
4	6.510	727	734	739	rBV	429400	572883	11.41%	5.198%
5	6.893	794	799	804	rVB	168816	203248	4.05%	1.844%
6	7.451	884	894	899	rBV	301386	388178	7.73%	3.522%
7	7.563	908	913	918	rVB	173029	211017	4.20%	1.915%
8	8.175	1009	1017	1027	rVB	221415	279888	5.57%	2.539%
9	9.251	1194	1200	1204	rVV	621920	780195	15.54%	7.079%
10	9.928	1310	1315	1325	rVB	236464	309174	6.16%	2.805%
11	10.716	1444	1449	1454	rBV	281668	356495	7.10%	3.235%
12	11.416	1564	1568	1576	rBV	198142	298713	5.95%	2.710%
13	11.945	1655	1658	1665	rBV2	96943	126458	2.52%	1.147%
14	12.463	1744	1746	1759	rVB2	64607	131358	2.62%	1.192%
15	12.763	1794	1797	1806	rVB	62241	96865	1.93%	0.879%
16	13.004	1834	1838	1847	rVB	475955	624294	12.43%	5.664%
17	13.504	1920	1923	1931	rVB	47863	77005	1.53%	0.699%
18	14.057	2010	2017	2023	rBV	255155	521890	10.39%	4.735%
19	14.216	2025	2044	2061	rVB3	926166	5021469	100.00%	45.561%
20	14.833	2146	2149	2159	rVB	56520	98378	1.96%	0.893%
21	15.539	2264	2269	2273	rVB	106248	151739	3.02%	1.377%

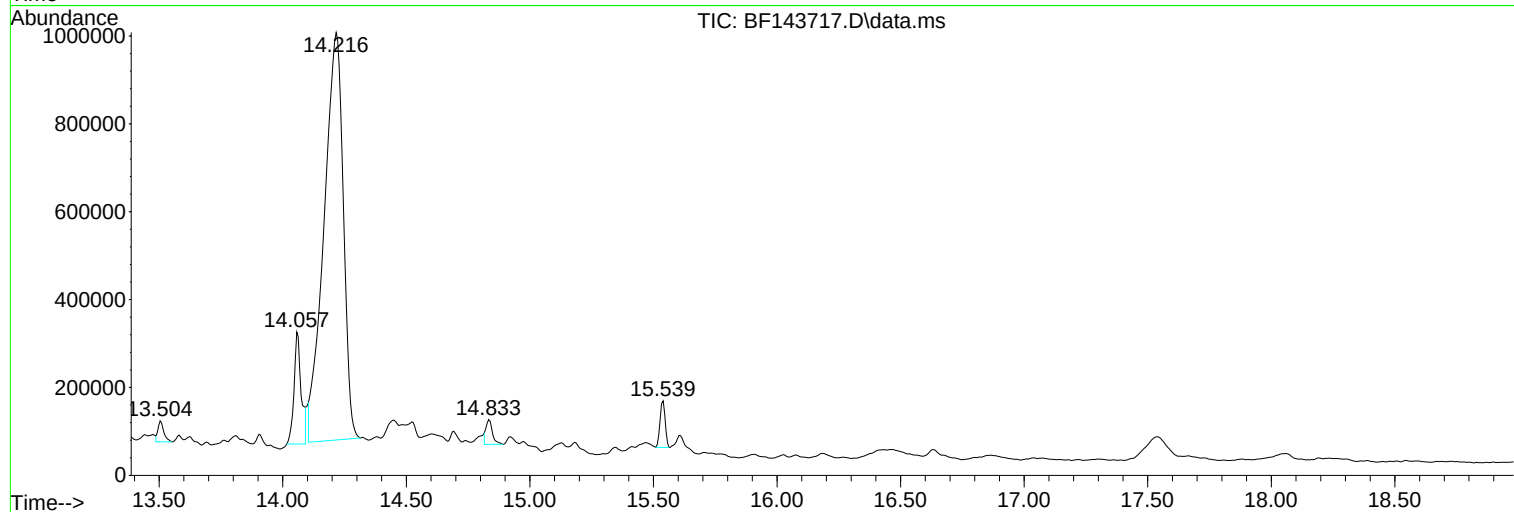
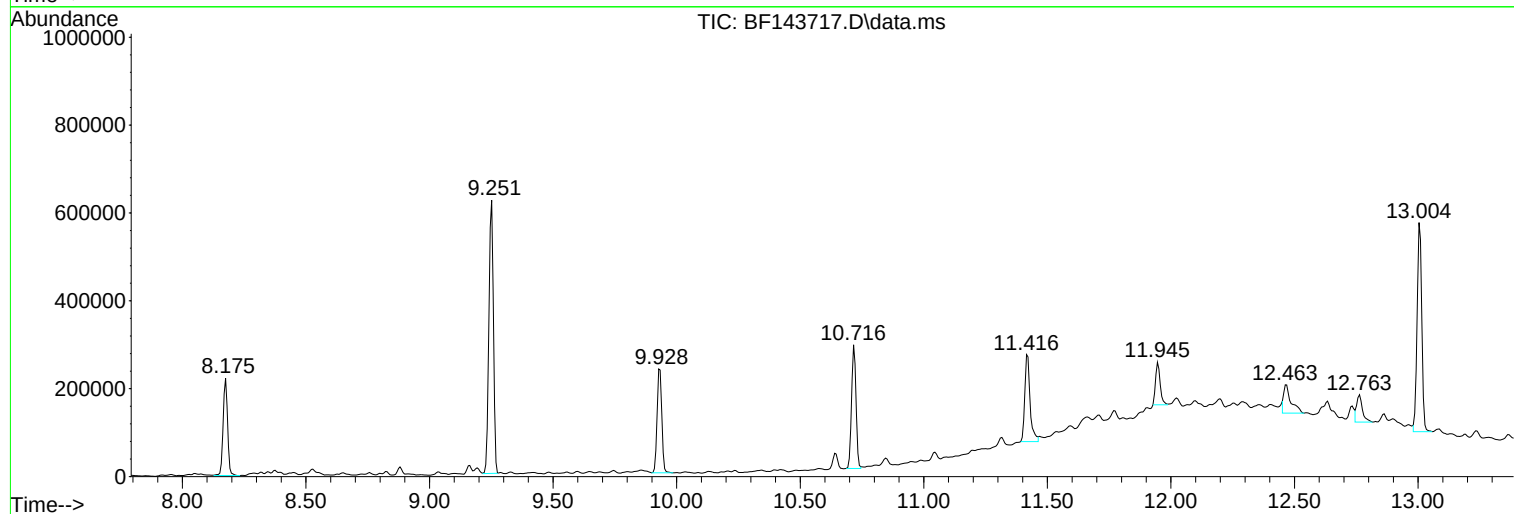
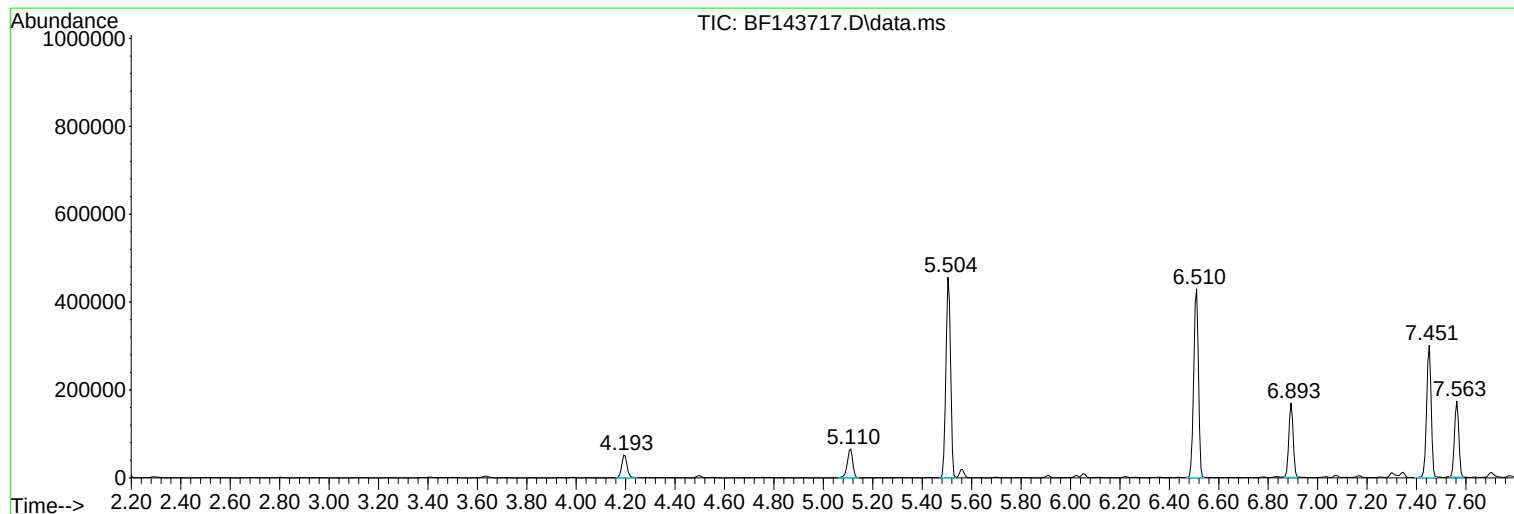
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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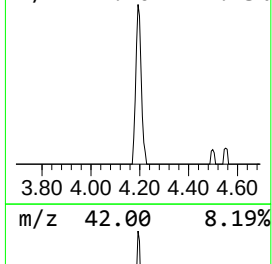
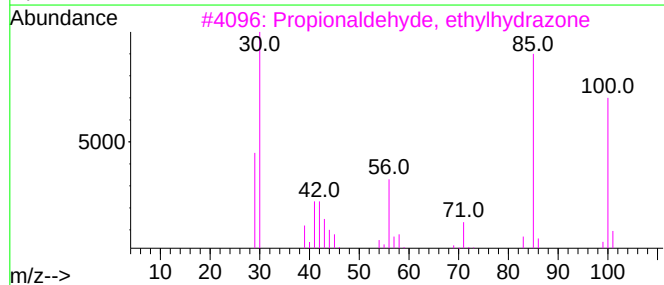
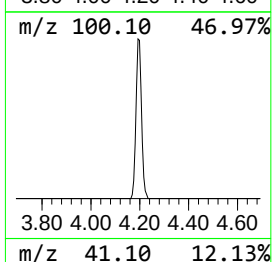
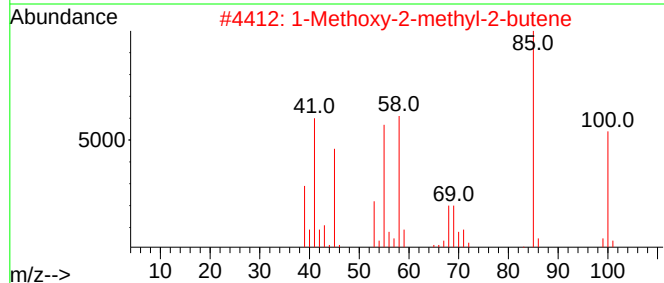
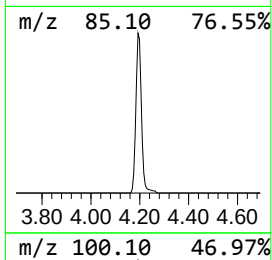
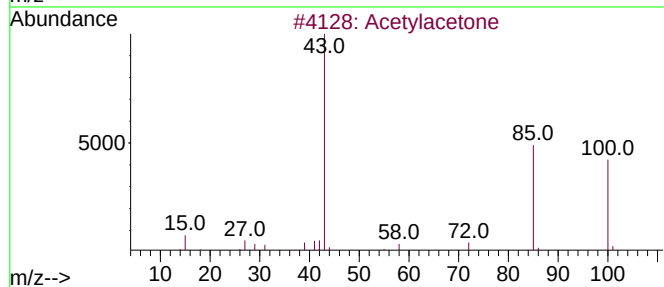
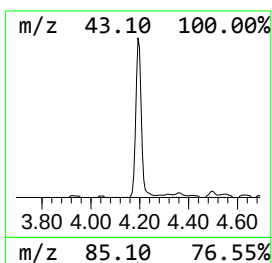
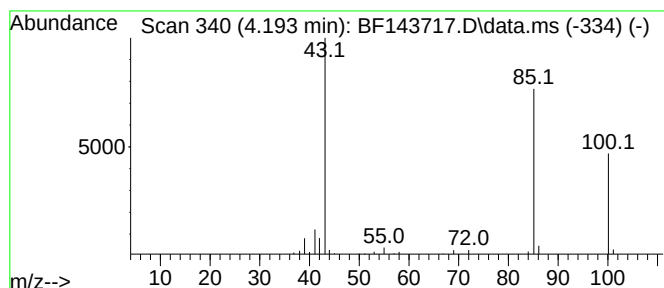
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Peak Number 1 Acetylacetone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.193	7.71 ng	78402	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetylacetone	100	C5H8O2	000123-54-6	83
2			1-Methoxy-2-methyl-2-butene	100	C6H12O	1000279-59-7	64
3			Propionaldehyde, ethylhydrazone	100	C5H12N2	007422-92-6	64
4			3-Penten-2-one, 4-(acetyloxy)-, ...	142	C7H10O3	038365-58-1	64
5			Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	42



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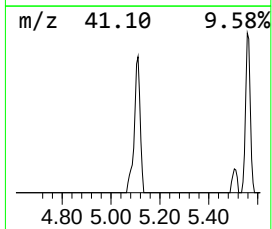
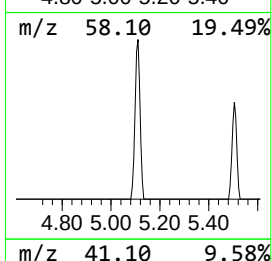
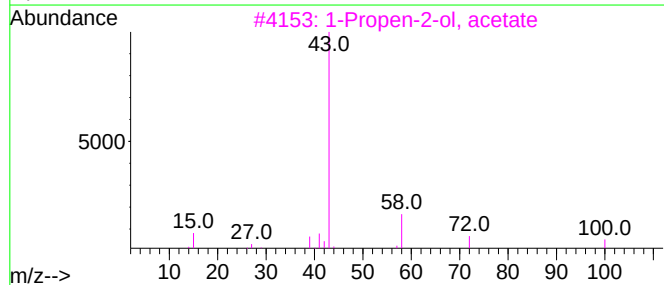
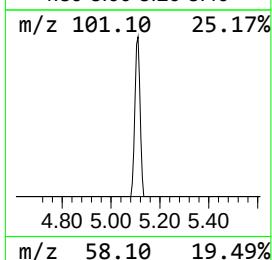
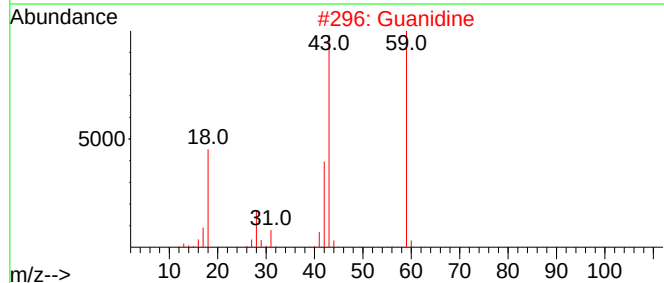
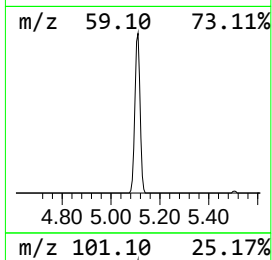
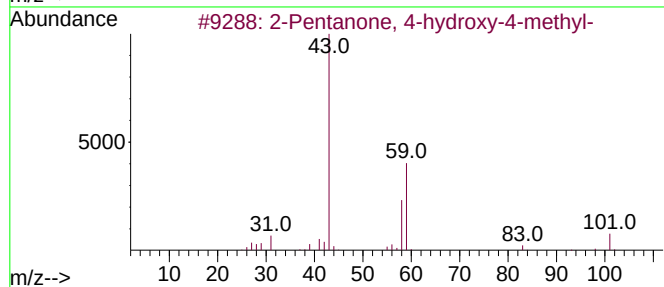
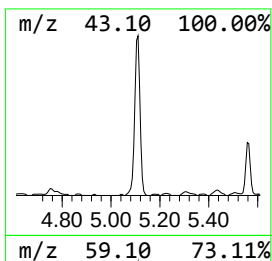
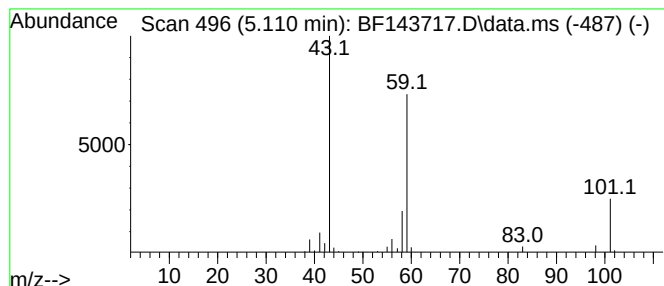
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	9.80 ng	99549	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Guanidine	59	CH5N3	000113-00-8	38
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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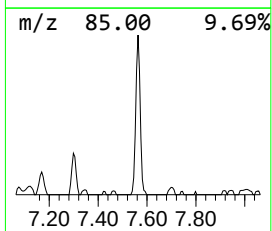
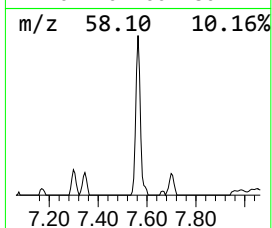
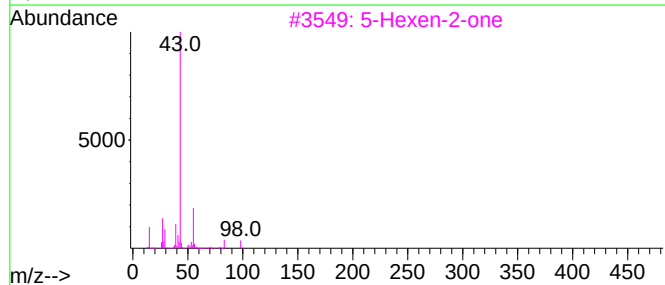
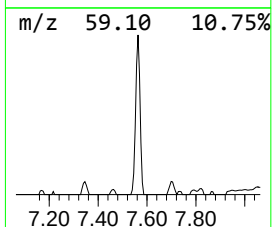
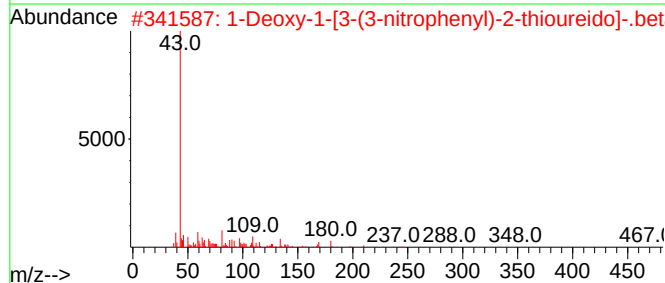
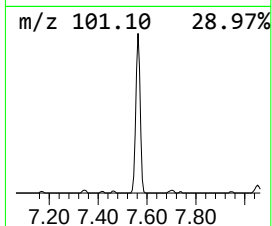
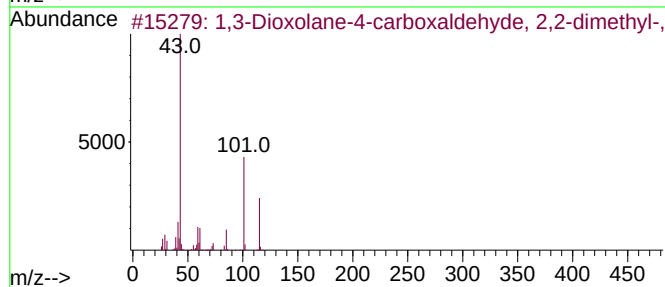
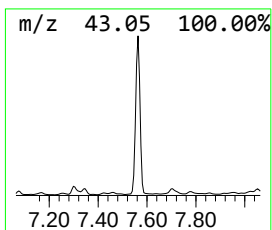
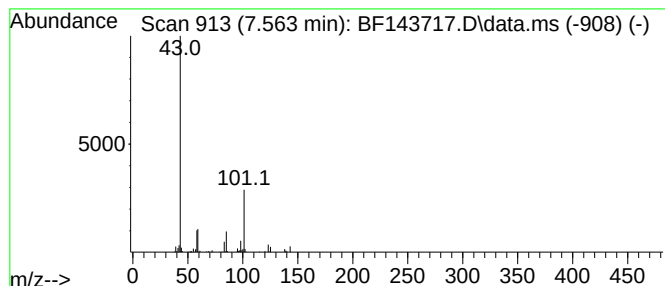
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Peak Number 3 unknown7.563 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	15.08 ng	211017	Naphthalene-d8	8.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane-4-carboxaldehyde, ...	130	C6H10O3	015186-48-8	25
2			1-Deoxy-1-[3-(3-nitrophenyl)-2-t...	527	C21H25N3O11S	1000223-13-3	12
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	9
5			5-Methyl-6,8-dioxa-3-thiabicyclo...	178	C6H10O4S	069697-61-6	9



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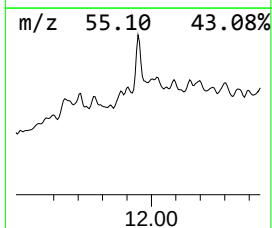
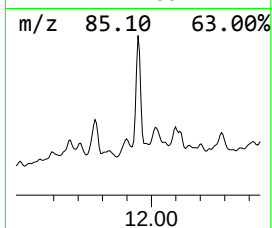
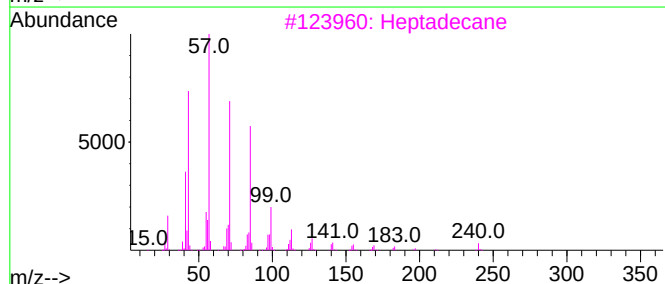
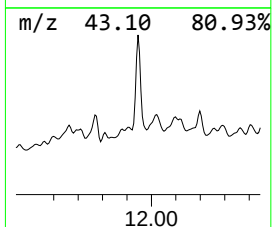
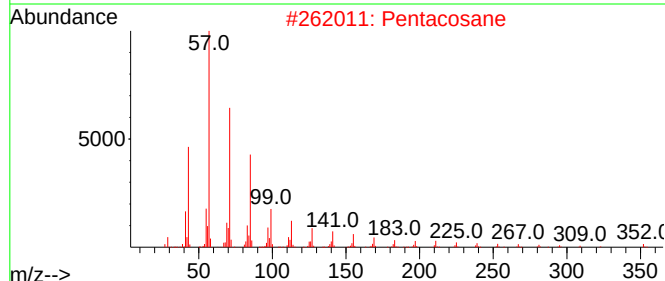
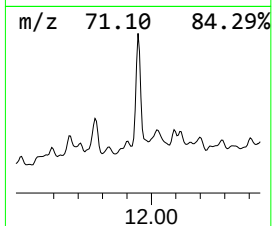
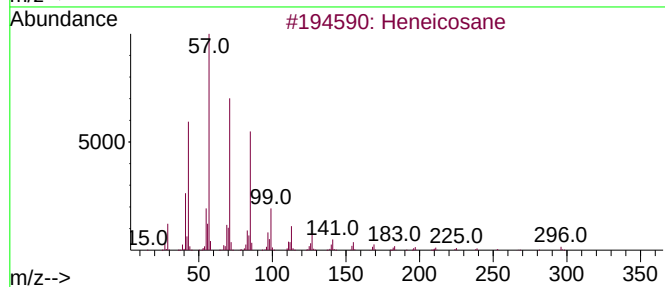
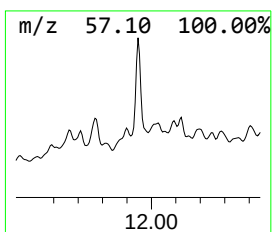
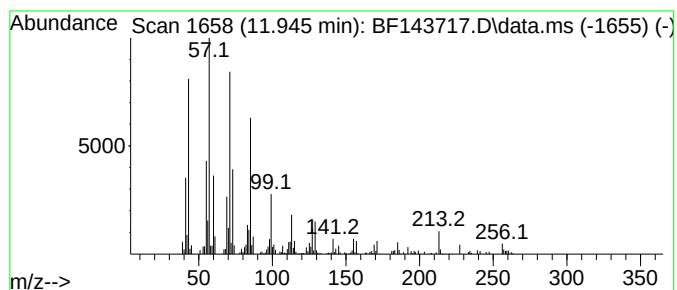
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Peak Number 4 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	8.47 ng	126458	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	68
2			Pentacosane	352	C25H52	000629-99-2	64
3			Heptadecane	240	C17H36	000629-78-7	64
4			Hexacosane	366	C26H54	000630-01-3	62
5			Heptacosane	380	C27H56	000593-49-7	58



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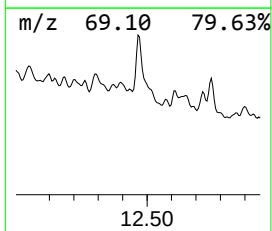
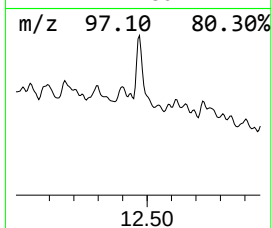
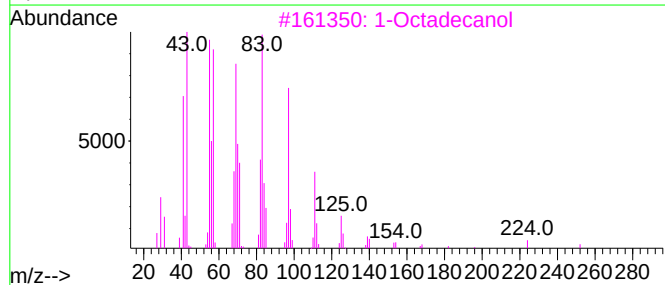
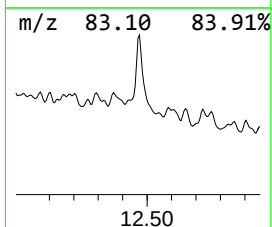
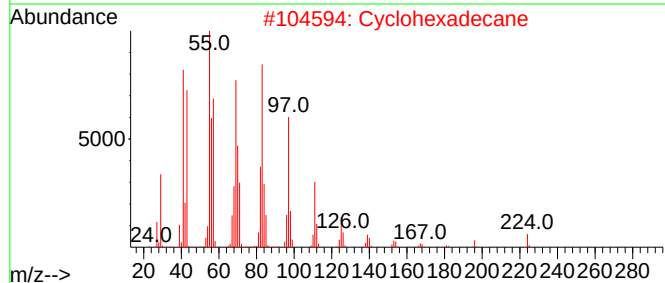
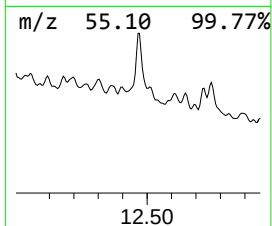
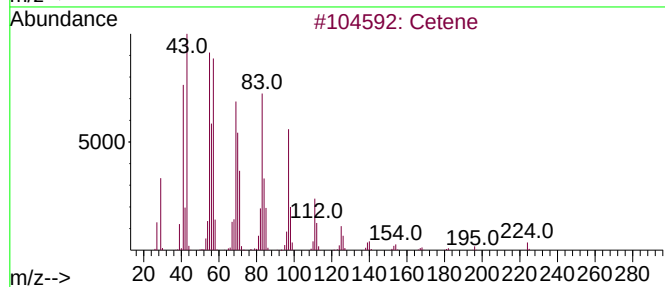
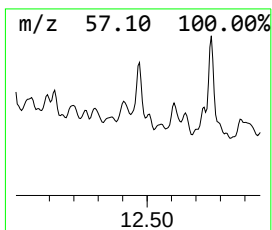
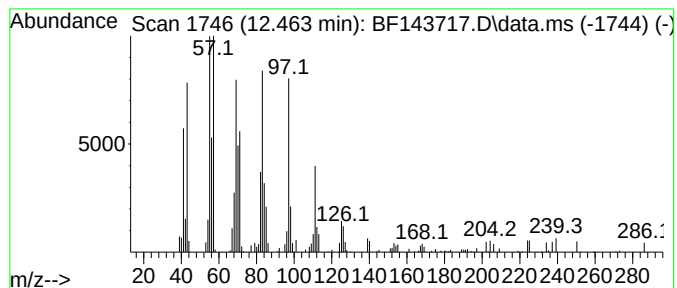
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Peak Number 5 Cetene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	8.79 ng	131358	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cetene	224	C16H32	000629-73-2	96
2			Cyclohexadecane	224	C16H32	000295-65-8	95
3			1-Octadecanol	270	C18H38O	000112-92-5	95
4			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	94
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	91



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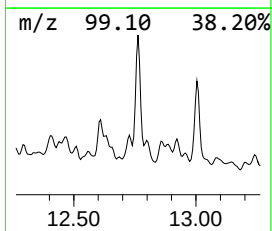
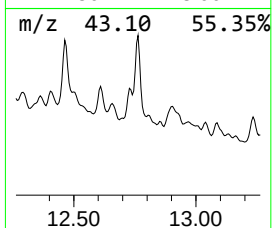
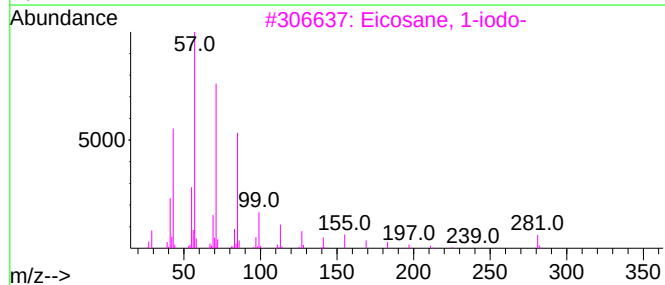
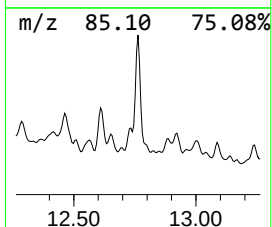
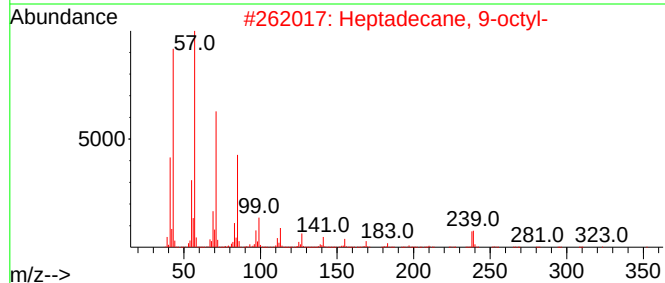
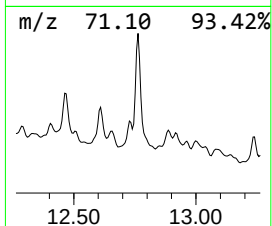
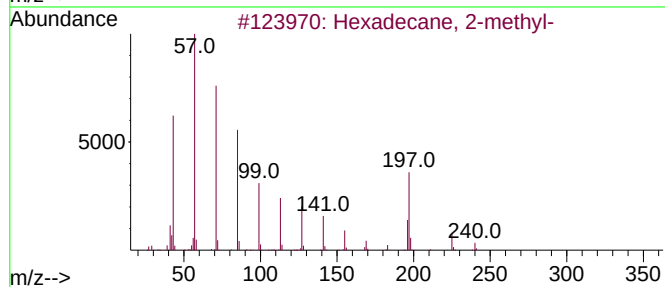
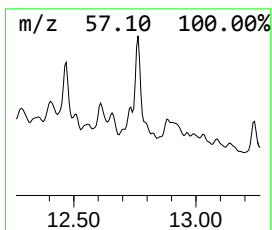
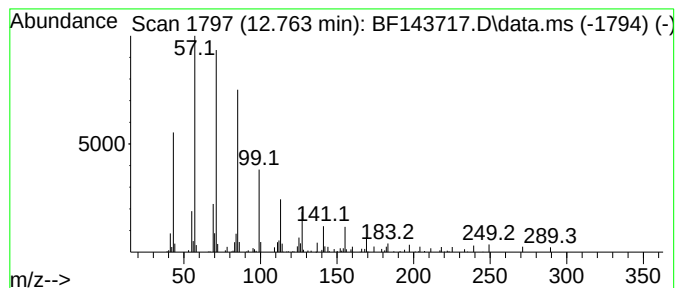
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.763	3.71 ng	96865	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	90
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	72
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	72
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143717.D
Acq On : 11 Sep 2025 20:27
Operator : RC/JU
Sample : Q3075-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-25-0259

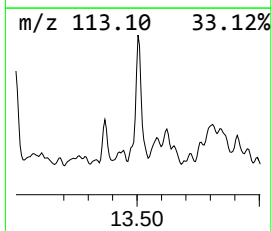
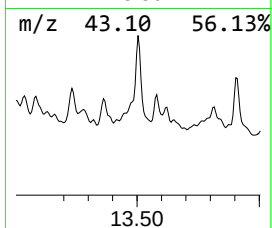
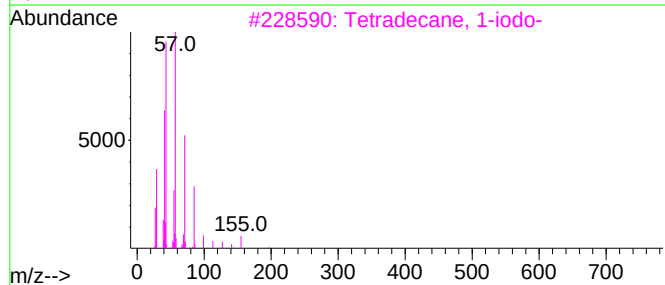
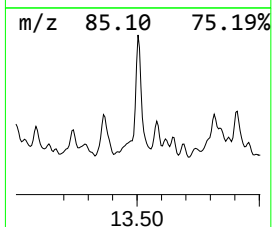
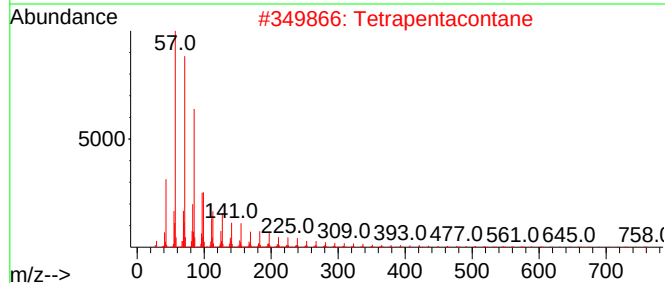
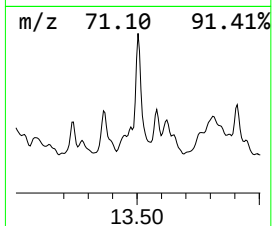
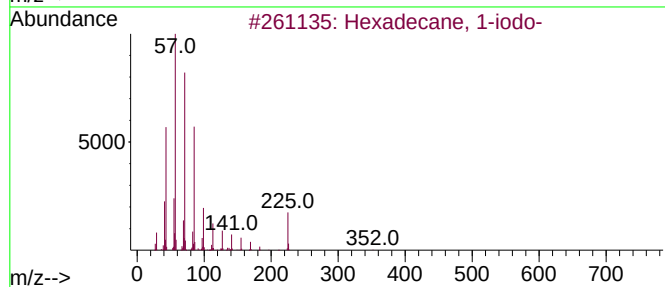
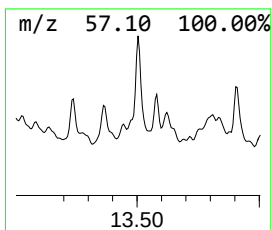
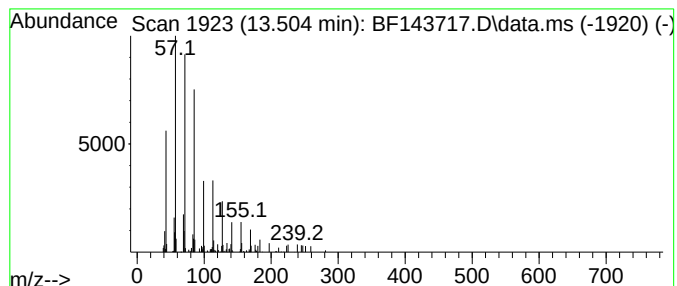
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	2.95 ng	77005	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72
2			Tetrapentacontane	759	C54H110	005856-66-6	72
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	59
4			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	59
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143717.D
Acq On : 11 Sep 2025 20:27
Operator : RC/JU
Sample : Q3075-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-25-0259

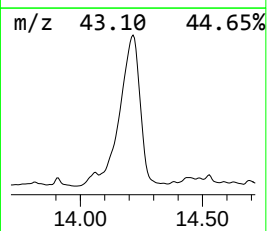
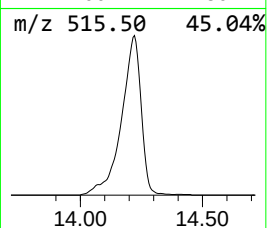
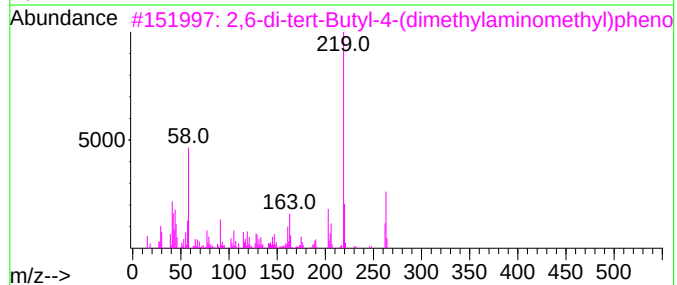
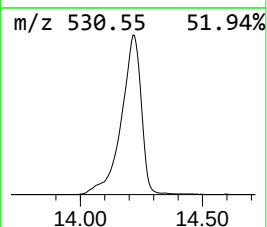
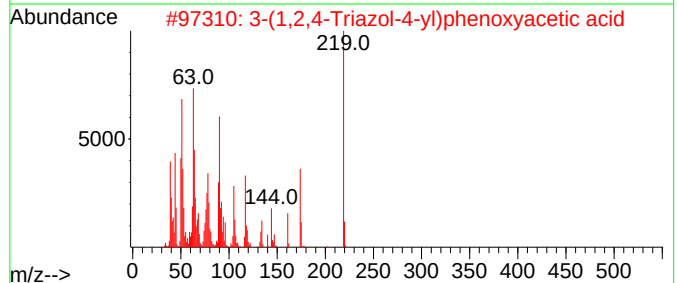
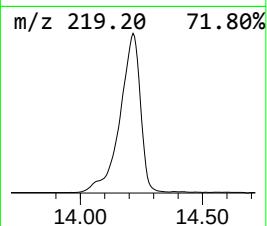
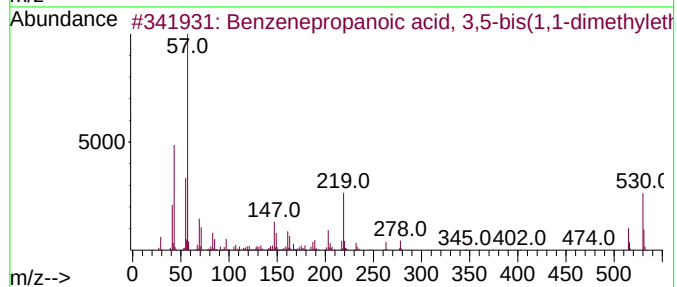
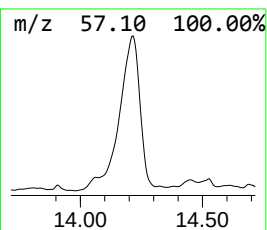
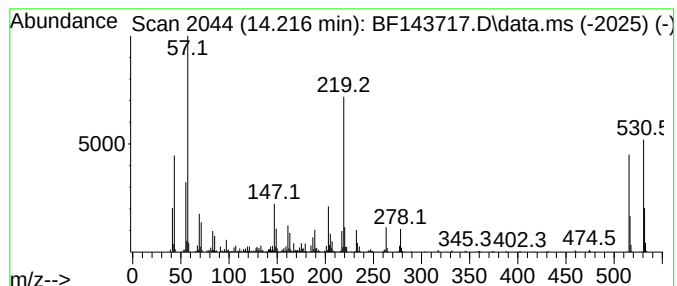
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzenepropanoic acid, 3,5-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.216	192.43 ng	5021470	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenepropanoic acid, 3,5-bis(1...	530	C35H62O3	002082-79-3	99
2			3-(1,2,4-Triazol-4-yl)phenoxyace...	219	C10H9N3O3	847606-79-5	11
3			2,6-di-tert-Butyl-4-(dimethylami...	263	C17H29NO	000088-27-7	10
4			Isophthalic acid, 2-nitro-5-fluo...	375	C19H18FNO6	1000344-41-9	10
5			4-(1H-Inden-1-ylidenemethyl)phen...	219	C16H13N	000487-61-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143717.D
Acq On : 11 Sep 2025 20:27
Operator : RC/JU
Sample : Q3075-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-25-0259

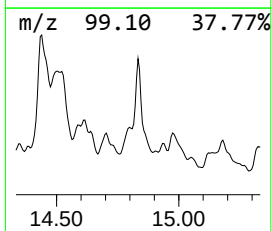
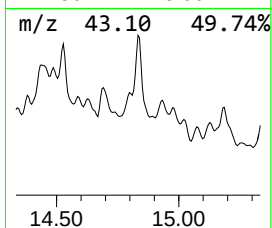
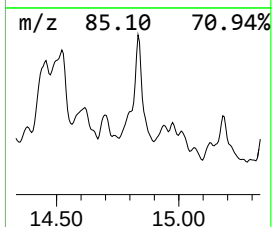
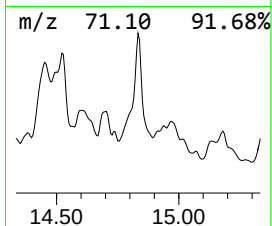
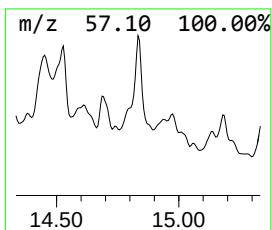
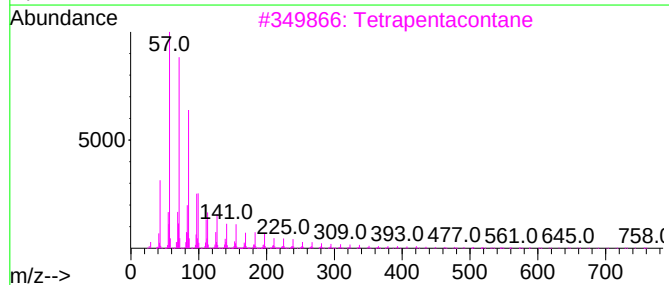
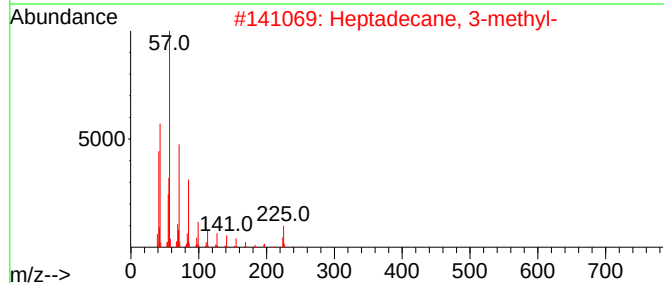
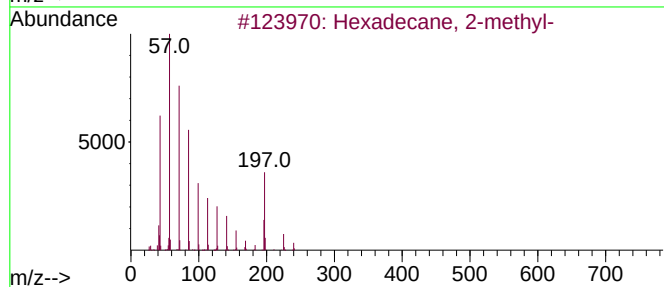
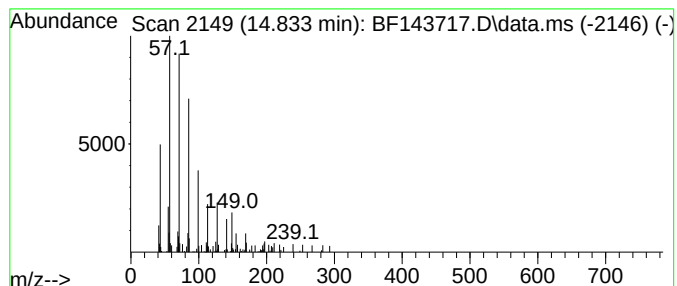
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.833 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	12.97 ng	98378	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	86
2			Heptadecane, 3-methyl-	254	C18H38	006418-44-6	78
3			Tetrapentacontane	759	C54H110	005856-66-6	78
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	64
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143717.D
Acq On : 11 Sep 2025 20:27
Operator : RC/JU
Sample : Q3075-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-25-0259

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.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
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2-Pentanone, 4-...	5.110	9.8	ng	99549	1	6.893	203248	20.0
unknown7.563	7.563	15.1	ng	211017	2	8.175	279888	20.0
Heneicosane	11.945	8.5	ng	126458	4	11.416	298713	20.0
Cetene	12.463	8.8	ng	131358	4	11.416	298713	20.0
Hexadecane, 2-m...	12.763	3.7	ng	96865	5	14.057	521890	20.0
Hexadecane, 1-i...	13.504	3.0	ng	77005	5	14.057	521890	20.0
Benzenepropanoi...	14.216	192.4	ng	5021470	5	14.057	521890	20.0
unknown14.833	14.833	13.0	ng	98378	6	15.539	151739	20.0