

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012125\
 Data File : BF141234.D
 Acq On : 21 Jan 2025 14:28
 Operator : RC/JU
 Sample : Q1132-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HD-1-011725

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-BF011025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141234.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	19	rVB	53657	92042	3.00%	0.388%
2	5.010	485	496	504	rBV	184294	293995	9.58%	1.238%
3	5.416	559	565	570	rBV	1995933	2598960	84.70%	10.946%
4	6.434	732	738	753	rVB	1912947	2622024	85.45%	11.044%
5	6.804	796	801	806	rBV	752179	915568	29.84%	3.856%
6	7.363	885	896	901	rBV	1346315	1723673	56.17%	7.260%
7	7.463	905	913	927	rVB	148258	307986	10.04%	1.297%
8	7.622	935	940	946	rVB	66076	89366	2.91%	0.376%
9	8.087	1013	1019	1024	rBV	922162	1181343	38.50%	4.976%
10	8.304	1051	1056	1060	rVB3	23155	31319	1.02%	0.132%
11	9.163	1196	1202	1207	rBV	2385323	3068455	100.00%	12.924%
12	9.563	1265	1270	1273	rBV4	21701	32511	1.06%	0.137%
13	9.734	1290	1299	1305	rBV	73186	144962	4.72%	0.611%
14	9.839	1311	1317	1322	rBV	987408	1216963	39.66%	5.126%
15	10.551	1434	1438	1443	rBV	148044	184723	6.02%	0.778%
16	10.628	1445	1451	1456	rBV	1352027	1700044	55.40%	7.160%
17	10.757	1468	1473	1480	rVB2	51960	87110	2.84%	0.367%
18	11.228	1550	1553	1558	rVB	31321	42560	1.39%	0.179%
19	11.328	1565	1570	1577	rBV	831525	1086797	35.42%	4.577%
20	11.563	1607	1610	1617	rVB4	29236	49918	1.63%	0.210%
21	11.857	1655	1660	1670	rBV	568126	811989	26.46%	3.420%
22	12.116	1700	1704	1708	rBV2	38377	56756	1.85%	0.239%
23	12.539	1773	1776	1778	rBV	60729	76520	2.49%	0.322%
24	12.645	1789	1794	1801	rBV	371017	576061	18.77%	2.426%
25	12.769	1812	1815	1822	rVB	47311	64152	2.09%	0.270%
26	12.916	1835	1840	1847	rVB	2015742	2529801	82.45%	10.655%
27	13.827	1992	1995	2003	rVB4	131936	220345	7.18%	0.928%
28	13.969	2015	2019	2026	rBV	733530	1019305	33.22%	4.293%
29	15.445	2267	2270	2281	rVB	504828	917438	29.90%	3.864%

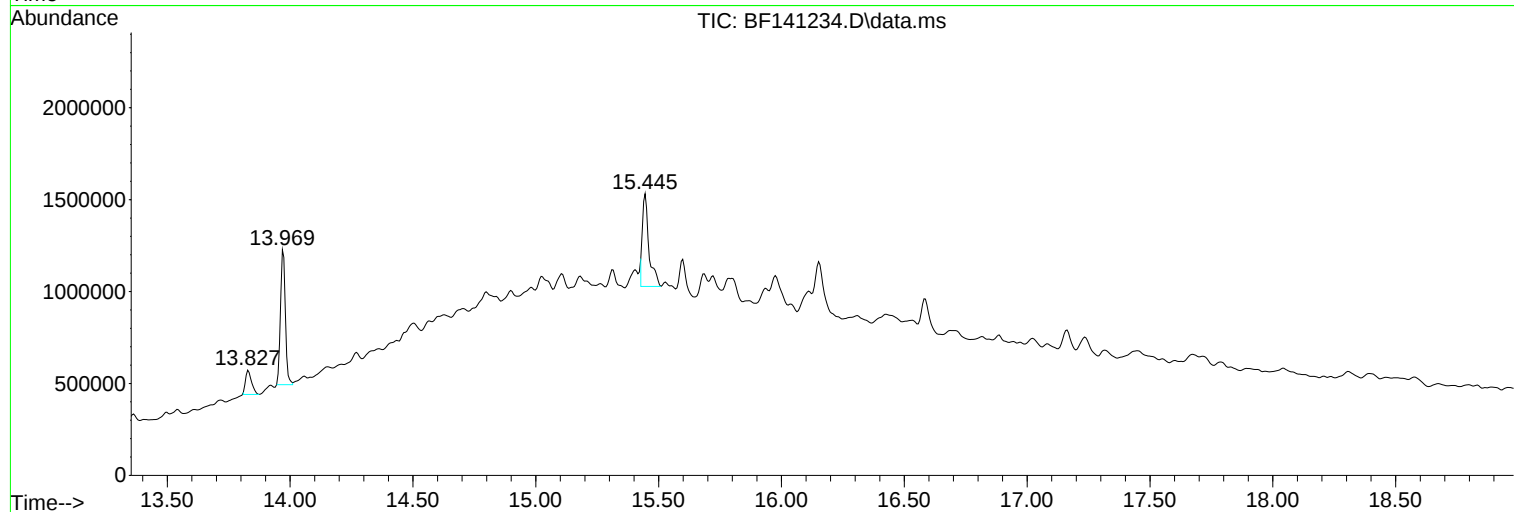
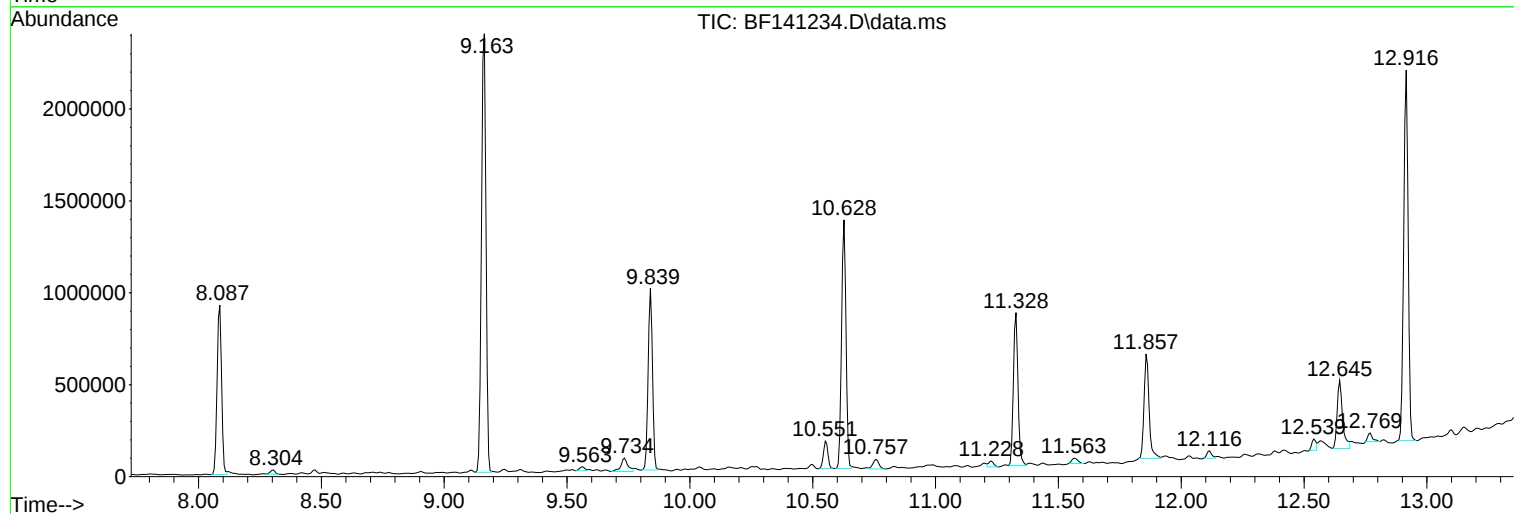
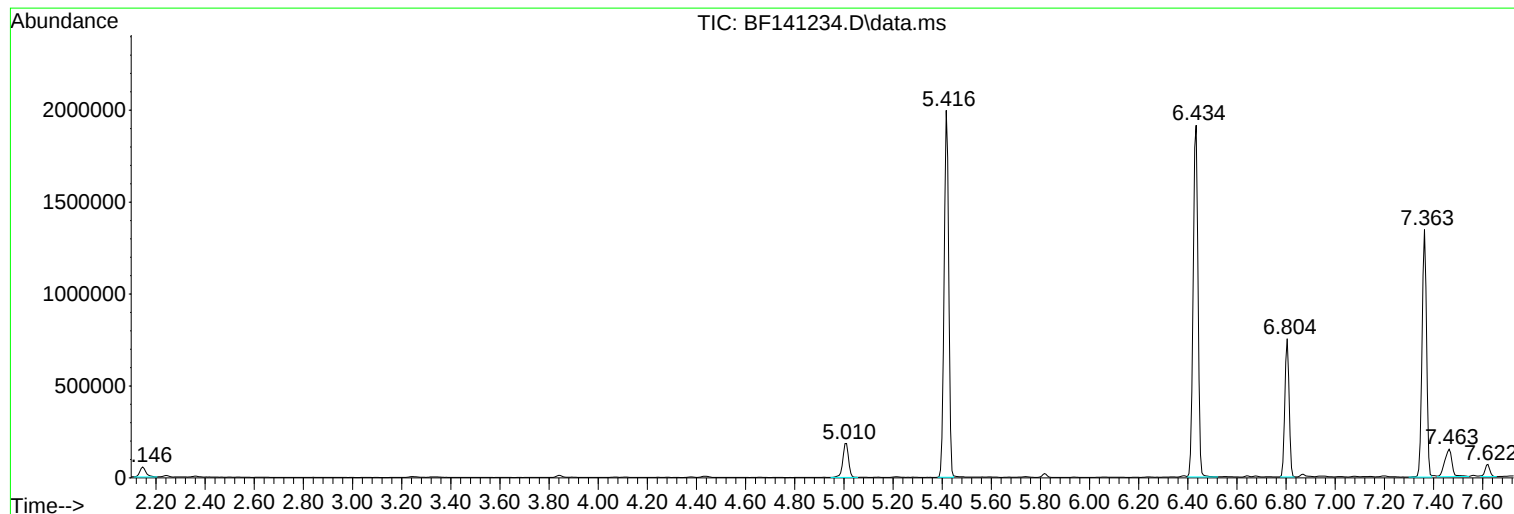
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Instrument :
BNA_F
ClientSampleId :
HD-1-011725

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.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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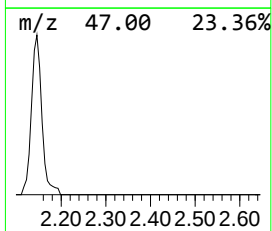
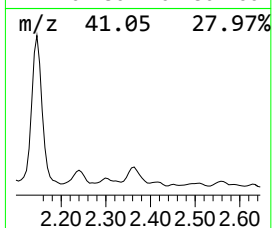
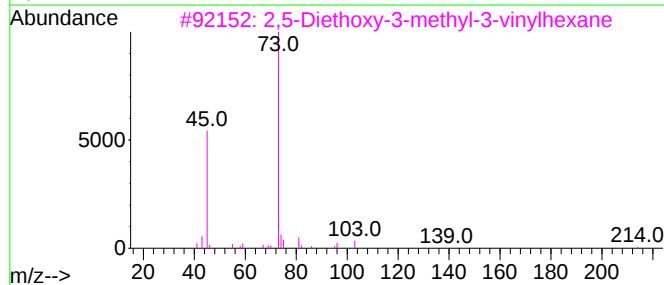
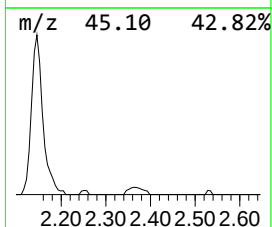
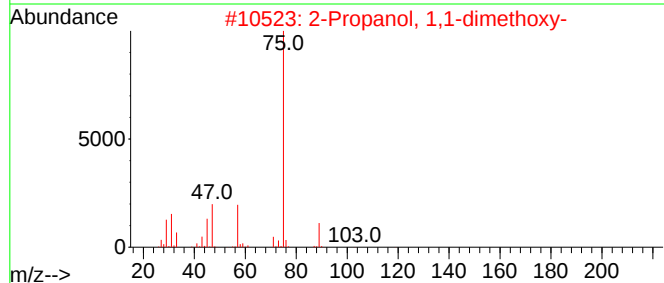
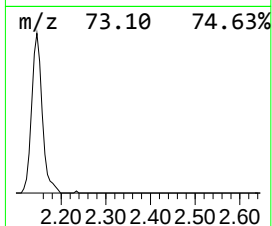
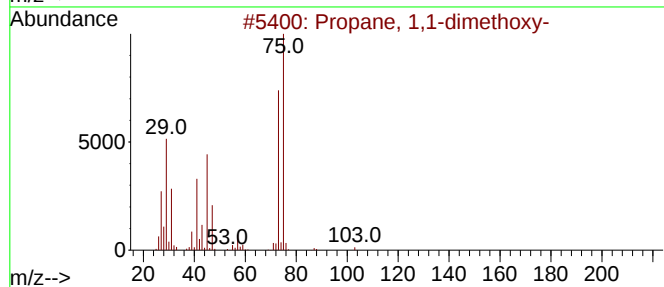
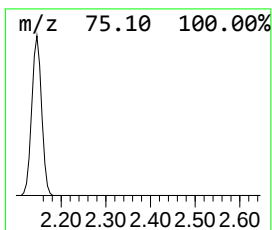
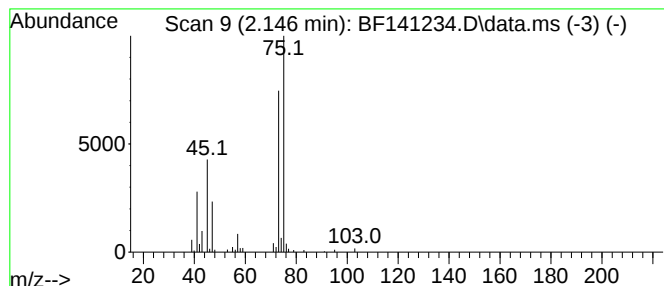
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	2.01 ng	92042	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	40
3			2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	16
4			(Methoxymethyl)trimethylsilane	118	C5H14OSi	014704-14-4	12
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10



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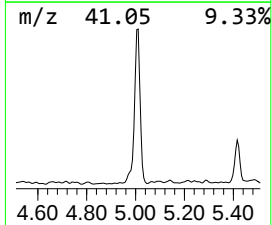
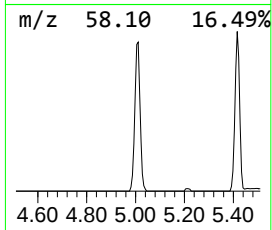
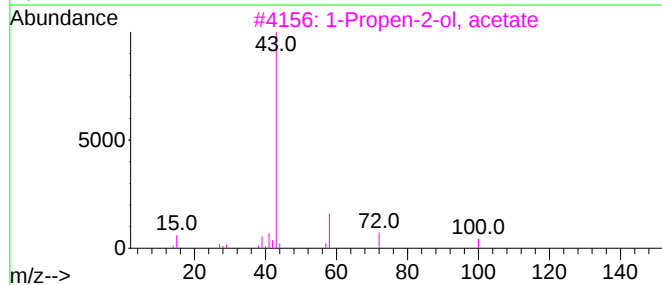
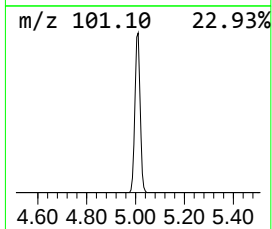
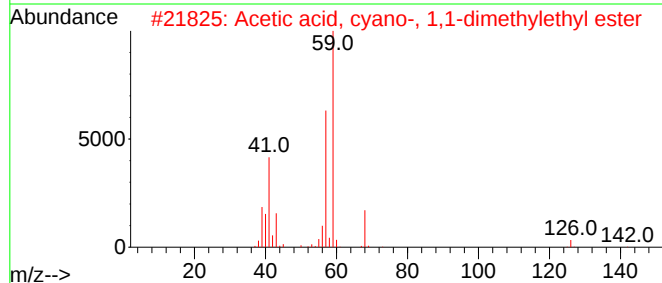
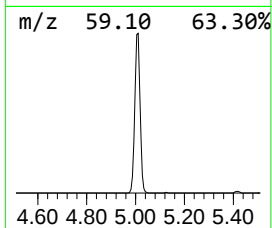
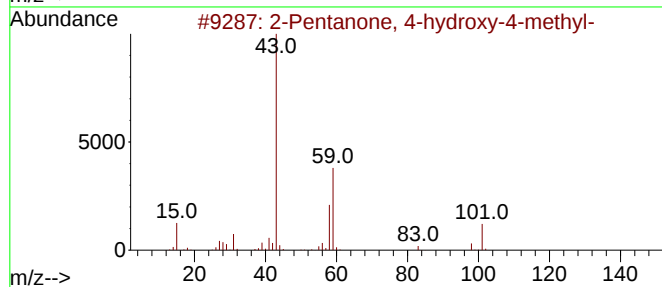
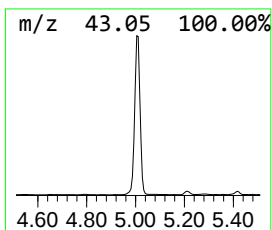
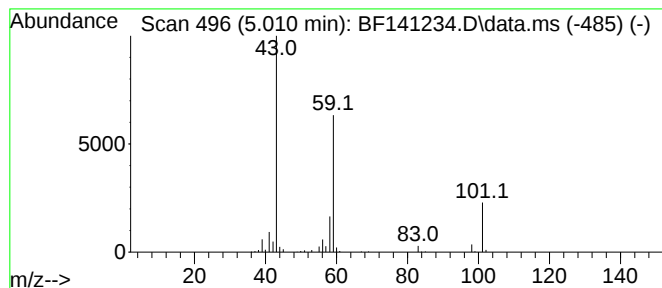
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.010	6.42 ng	293995	1,4-Dichlorobenzene-d4			6.804
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	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
4	5-Hexen-2-one		98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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Instrument :
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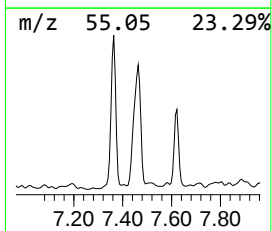
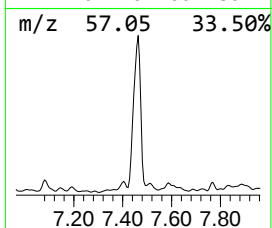
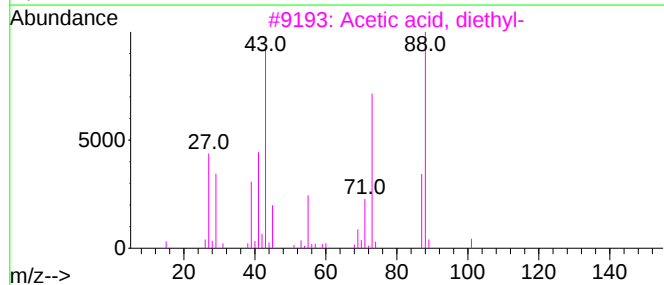
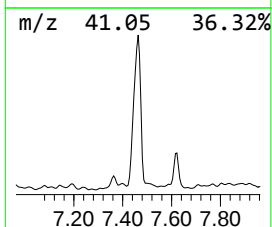
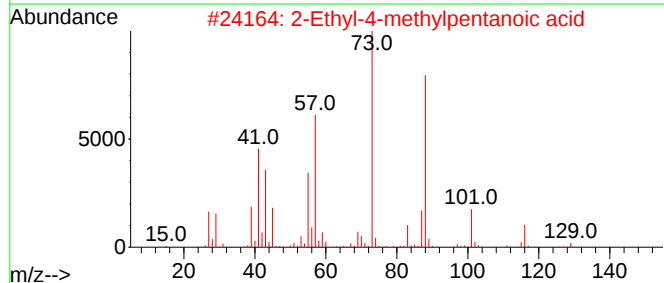
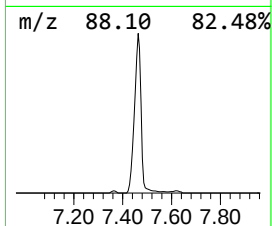
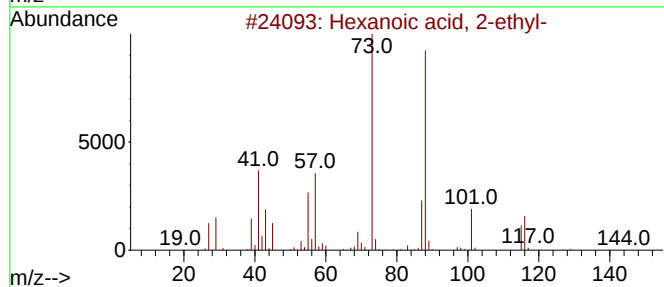
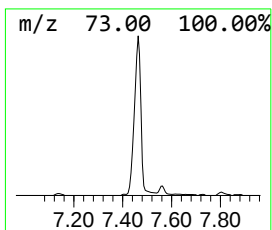
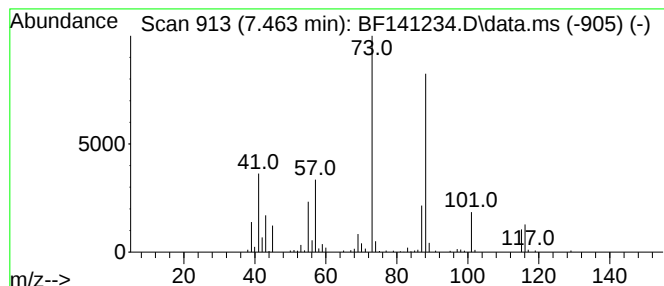
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.463	5.21 ng	307986	Naphthalene-d8	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	91
2			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	56
3			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	45
4			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
5			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42



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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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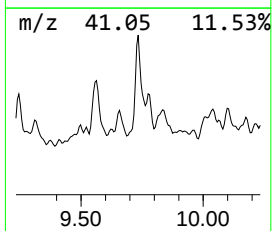
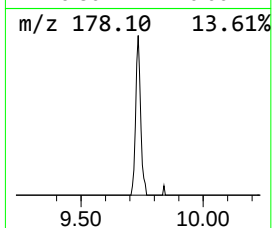
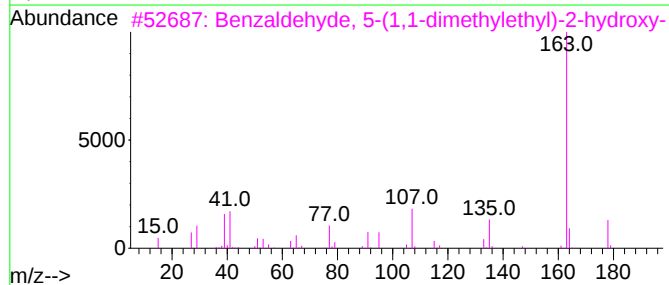
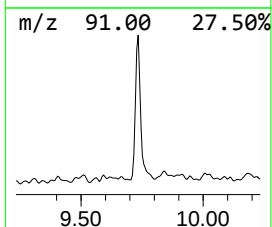
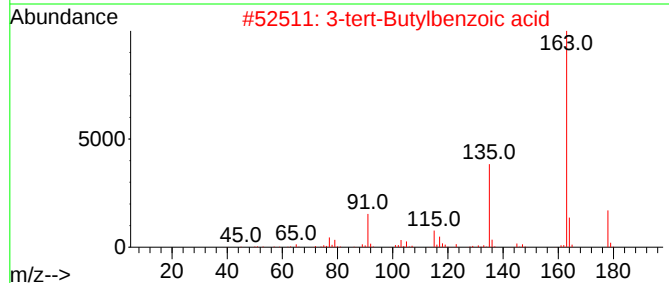
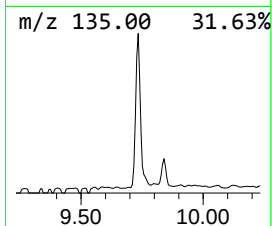
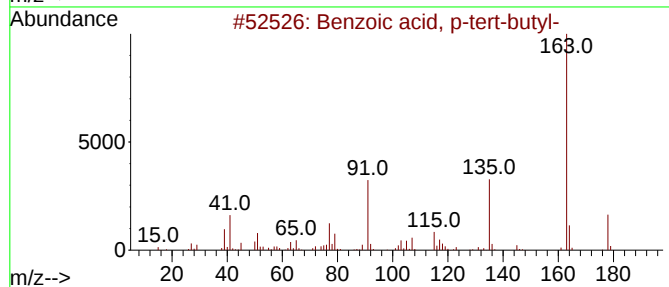
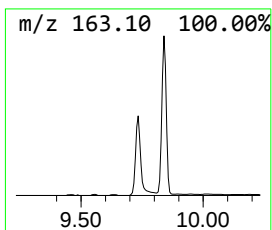
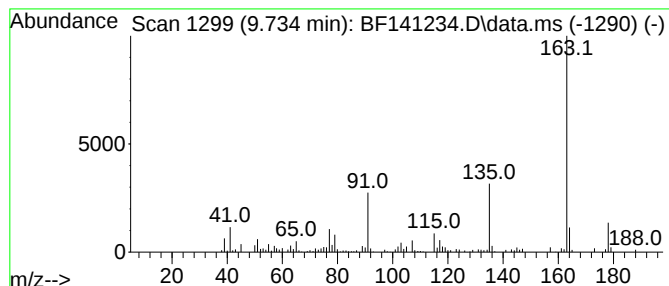
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Peak Number 4 Benzoic acid, p-tert-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.734	2.38 ng	144962	Acenaphthene-d10	9.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2			3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	94
3			Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	72
4			2-tert-Butyl-4-ethylphenol, 0-is...	264	C16H24O3	1000487-42-5	72
5			6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	72



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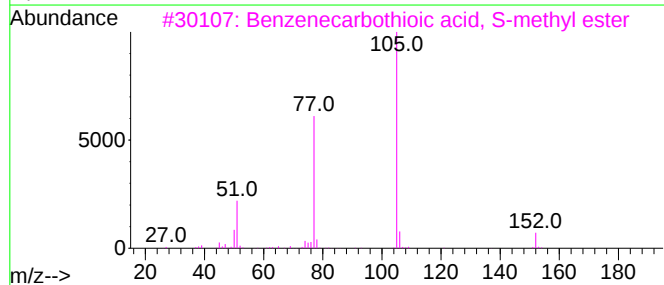
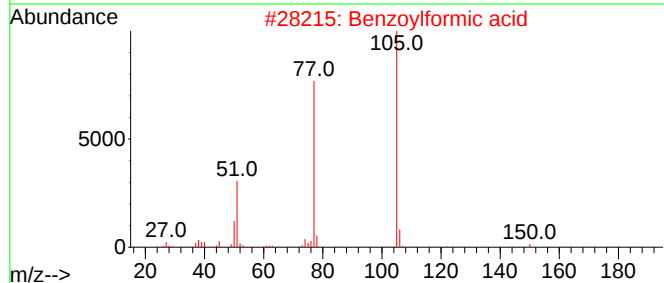
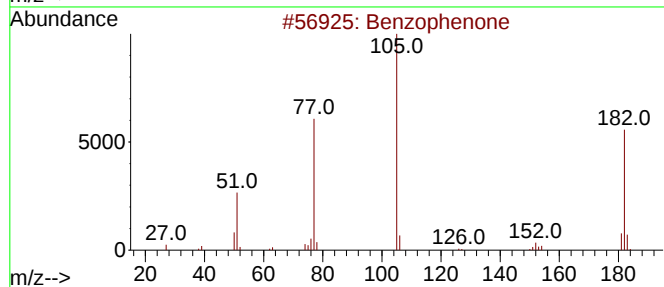
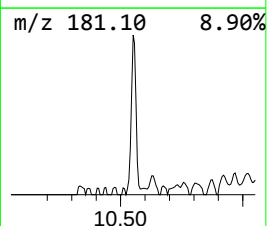
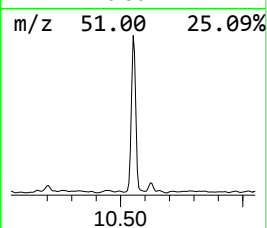
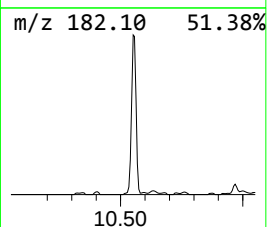
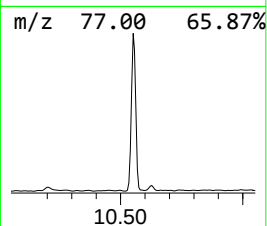
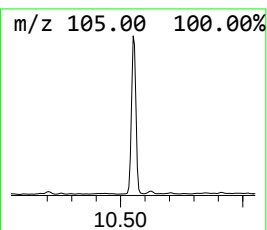
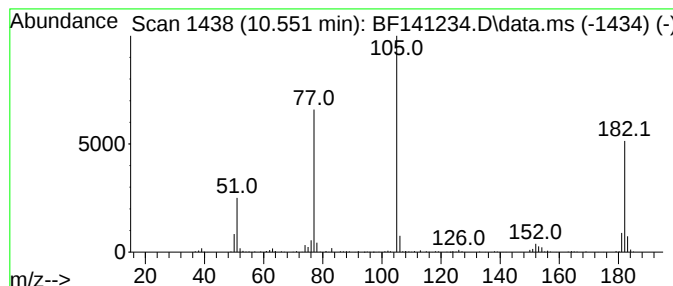
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Peak Number 5 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.551	3.04 ng	184723	Acenaphthene-d10	9.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoylformic acid	150	C8H6O3	000611-73-4	53
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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Misc :
ALS Vial : 8 Sample Multiplier: 1

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HD-1-011725

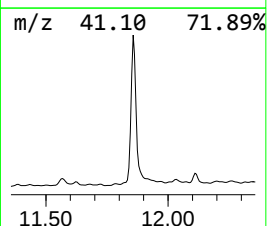
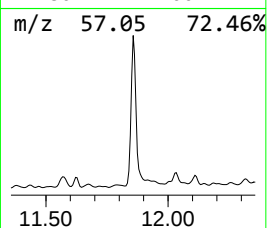
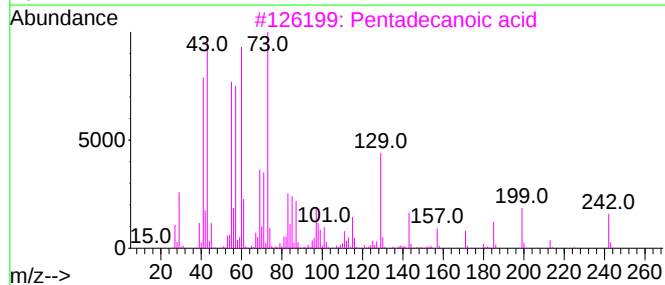
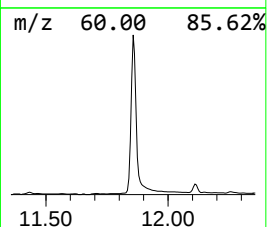
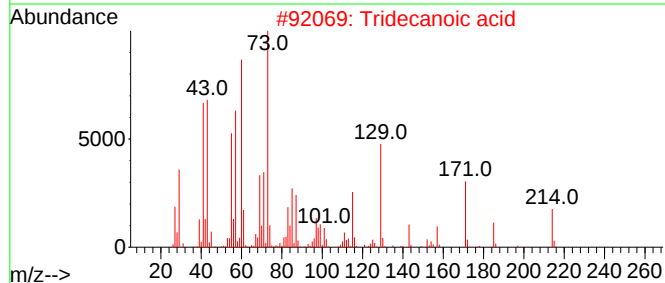
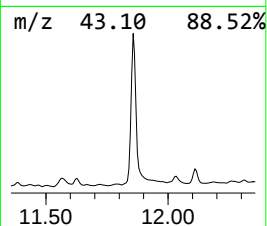
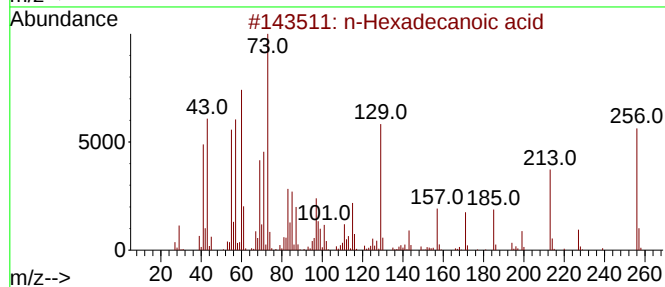
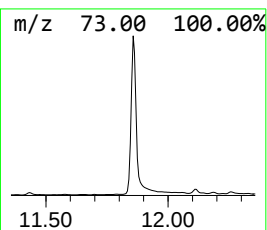
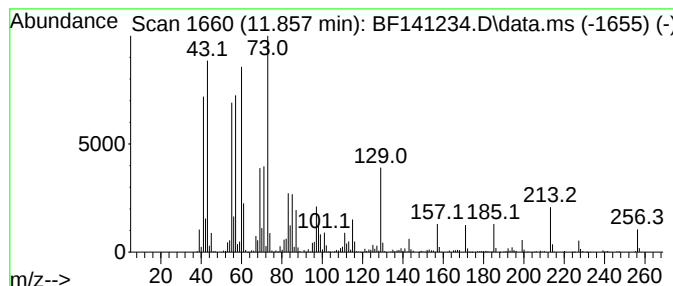
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	14.94 ng	811989	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012125\
Data File : BF141234.D
Acq On : 21 Jan 2025 14:28
Operator : RC/JU
Sample : Q1132-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-1-011725

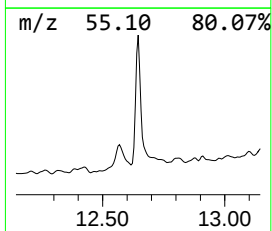
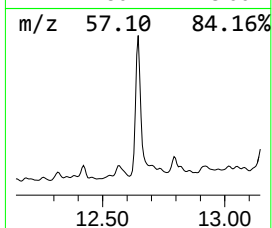
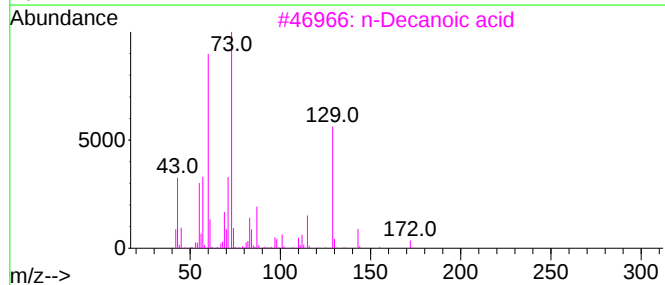
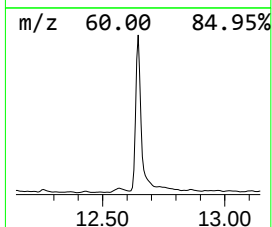
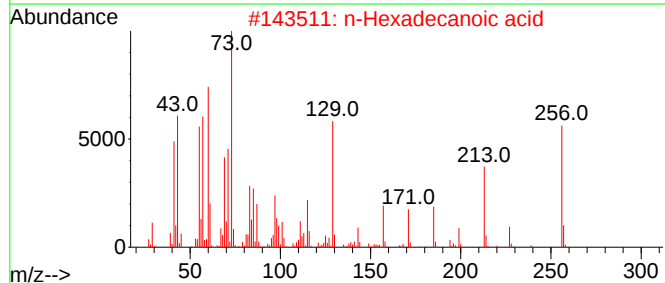
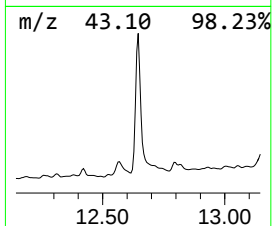
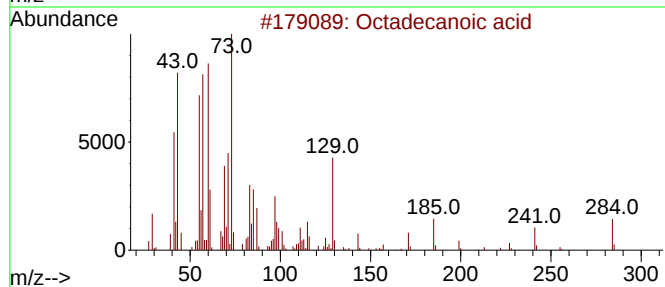
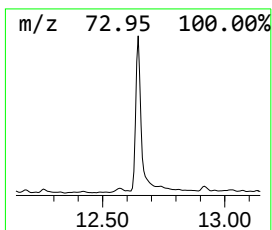
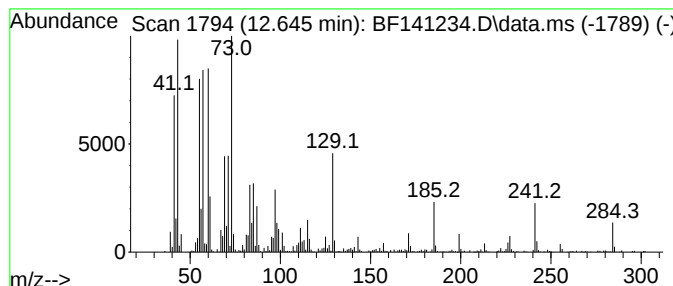
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	10.60 ng	576061	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			n-Decanoic acid	172	C10H20O2	000334-48-5	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012125\
Data File : BF141234.D
Acq On : 21 Jan 2025 14:28
Operator : RC/JU
Sample : Q1132-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-1-011725

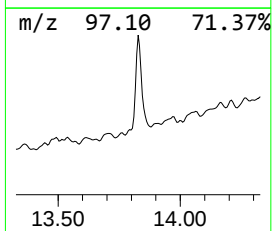
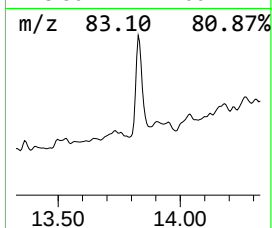
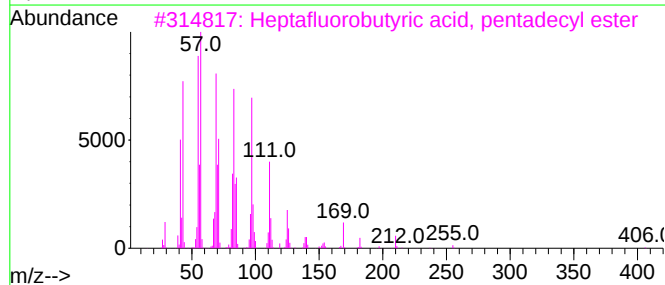
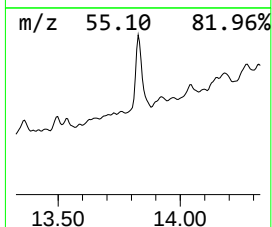
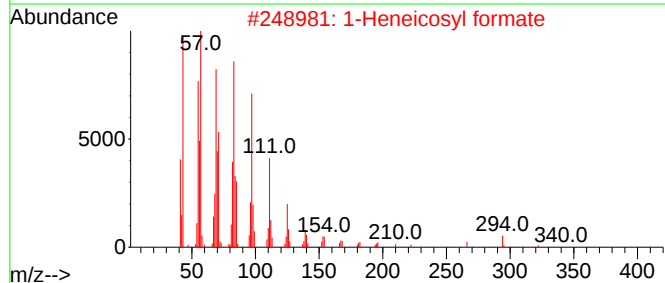
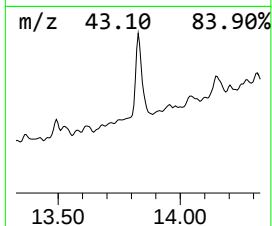
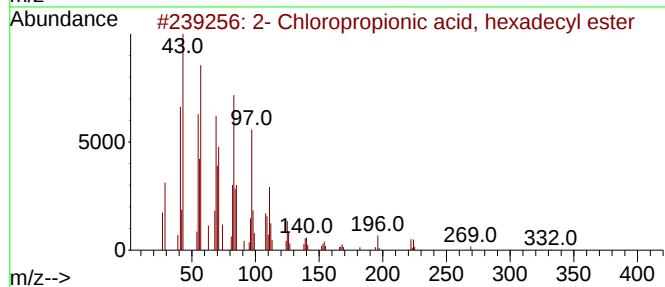
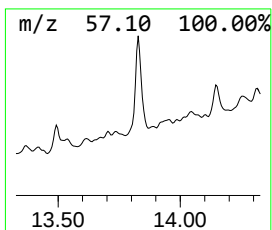
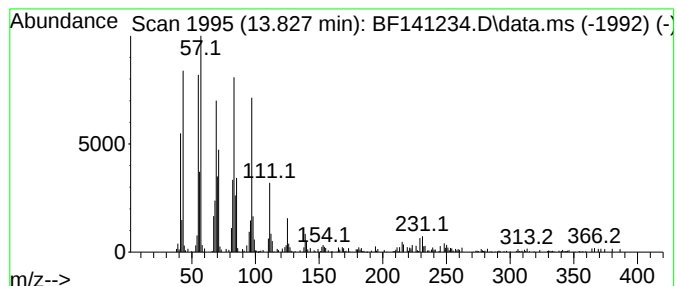
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2- Chloropropionic acid, he... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	4.32 ng	220345	Chrysene-d12	13.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	95
2	1-Heneicosyl	formate	340	C22H44O2	077899-03-7	95
3	Heptafluorobutyric	acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
5	Pentafluoropropionic	acid, penta...	374	C18H31F5O2	959092-08-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012125\
Data File : BF141234.D
Acq On : 21 Jan 2025 14:28
Operator : RC/JU
Sample : Q1132-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-1-011725

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-di...	2.146	2.0	ng	92042	1	6.804	915568	20.0
2-Pentanone, 4-...	5.010	6.4	ng	293995	1	6.804	915568	20.0
Hexanoic acid, ...	7.463	5.2	ng	307986	2	8.087	1181340	20.0
Benzoic acid, p...	9.734	2.4	ng	144962	3	9.839	1216960	20.0
Benzophenone	10.551	3.0	ng	184723	3	9.839	1216960	20.0
n-Hexadecanoic ...	11.857	14.9	ng	811989	4	11.328	1086800	20.0
Octadecanoic acid	12.645	10.6	ng	576061	4	11.328	1086800	20.0
2- Chloropropio...	13.827	4.3	ng	220345	5	13.969	1019310	20.0