

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
 Data File : BF138854.D
 Acq On : 07 Aug 2024 21:08
 Operator : RC/JU
 Sample : P3430-05
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 925-K1-WP0-0-0.25-073124

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-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138854.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.145	3	9	15	rVB	1737700	2745042	100.00%	23.560%
2	2.498	62	69	76	rBV	25368	47234	1.72%	0.405%
3	5.063	500	505	516	rVB	30346	43870	1.60%	0.377%
4	5.210	522	530	541	rBV	15995	49408	1.80%	0.424%
5	5.322	543	549	565	rVV3	9988	28690	1.05%	0.246%
6	5.469	569	574	585	rBV	568700	750412	27.34%	6.441%
7	6.481	741	746	770	rBV	400995	525425	19.14%	4.510%
8	6.839	802	807	812	rVB	222486	272357	9.92%	2.338%
9	7.257	870	878	890	rBV	30754	47730	1.74%	0.410%
10	7.404	896	903	914	rBV	732473	1026975	37.41%	8.814%
11	7.604	931	937	943	rBV	29942	55144	2.01%	0.473%
12	7.898	982	987	1005	rVB	46774	78660	2.87%	0.675%
13	8.116	1019	1024	1038	rVB	277774	363867	13.26%	3.123%
14	8.404	1069	1073	1076	rBV	32238	50652	1.85%	0.435%
15	8.433	1076	1078	1095	rVB	41268	75418	2.75%	0.647%
16	8.927	1158	1162	1181	rBV	55640	102072	3.72%	0.876%
17	9.192	1201	1207	1212	rBV	1445197	1854106	67.54%	15.914%
18	9.869	1317	1322	1327	rBV	318280	402791	14.67%	3.457%
19	10.663	1452	1457	1471	rBV	774513	1024535	37.32%	8.794%
20	11.357	1570	1575	1580	rBV	310416	378585	13.79%	3.249%
21	11.880	1659	1664	1681	rBV2	28363	54037	1.97%	0.464%
22	12.939	1838	1844	1849	rBV	976784	1227899	44.73%	10.539%
23	13.839	1991	1997	2010	rBV	20194	47152	1.72%	0.405%
24	13.998	2019	2024	2030	rVB	144546	194490	7.09%	1.669%
25	15.456	2266	2272	2283	rBV	133422	204496	7.45%	1.755%

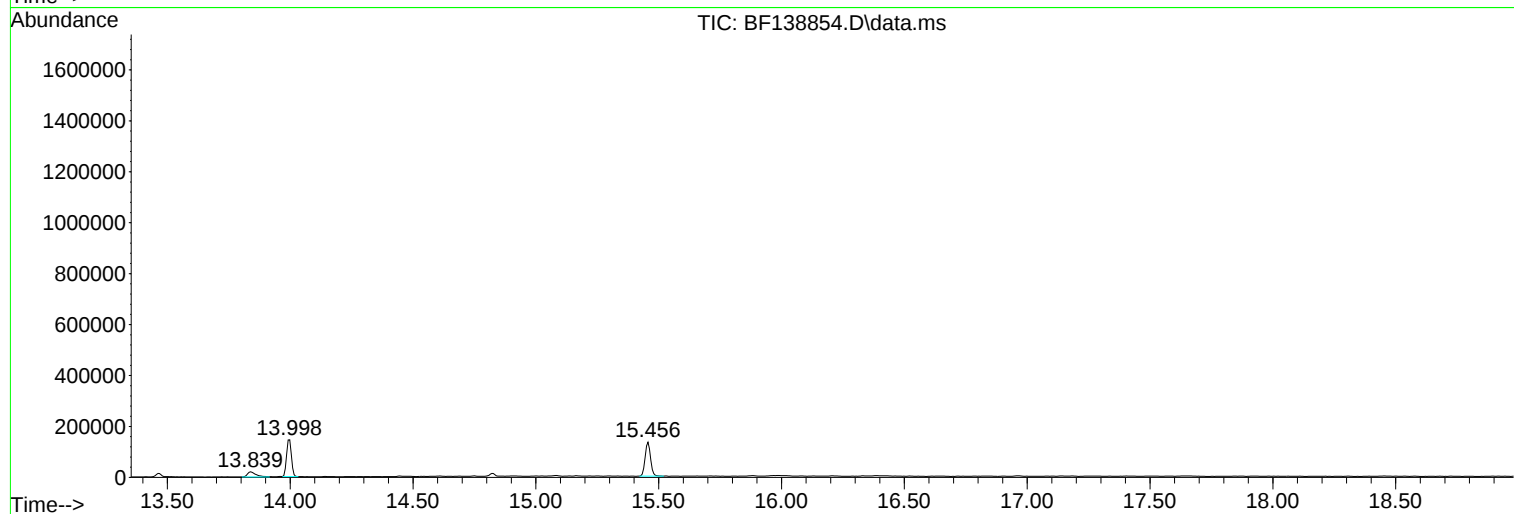
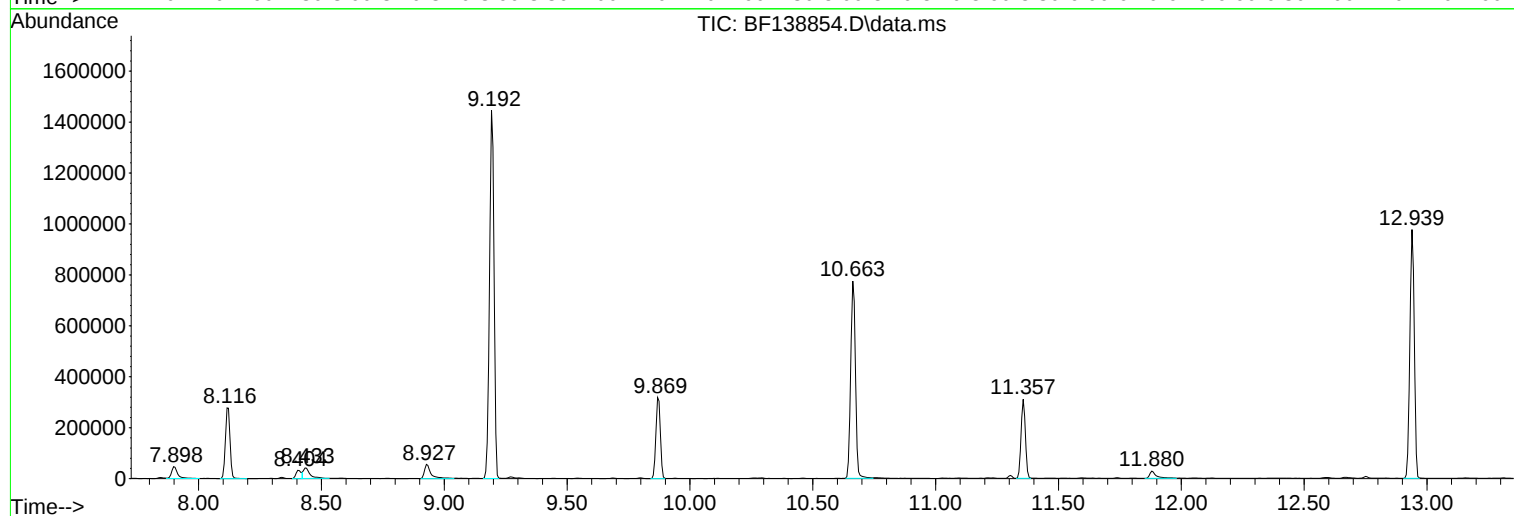
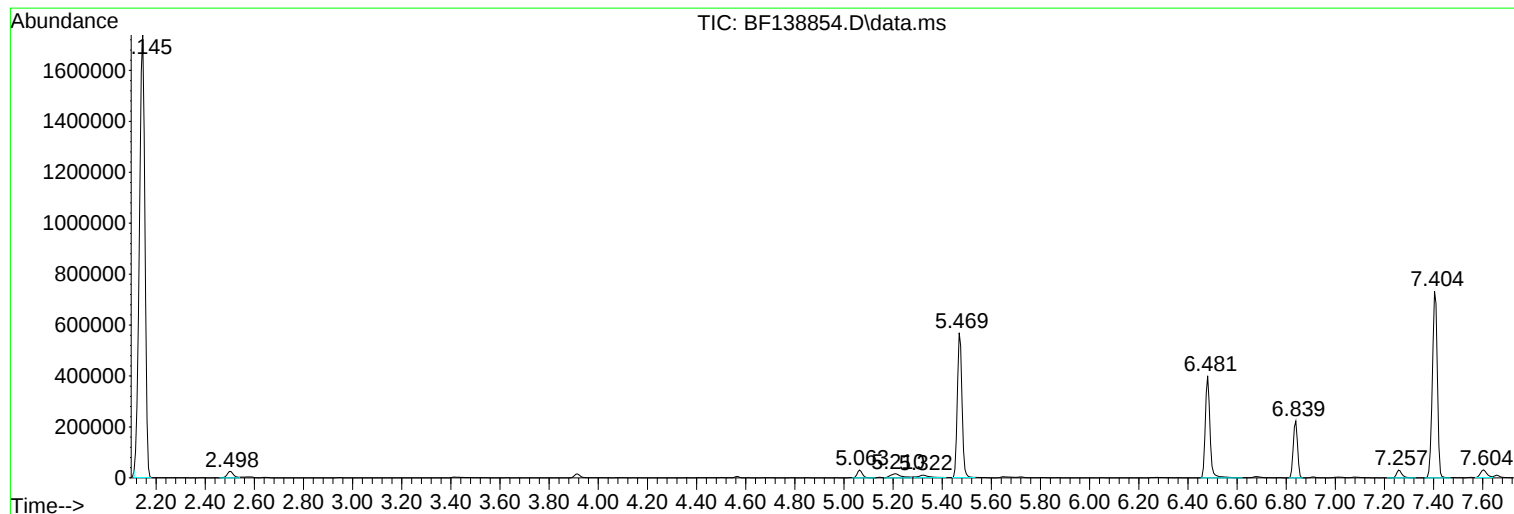
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ClientSampleId :
925-K1-WP0-0-0.25-073124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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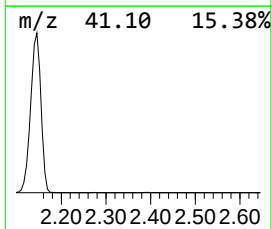
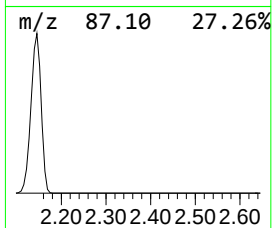
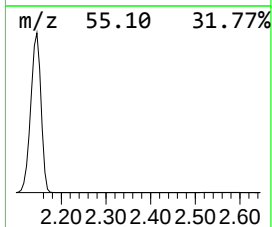
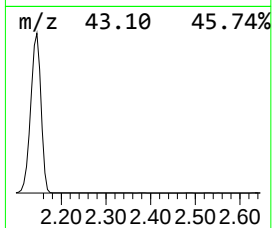
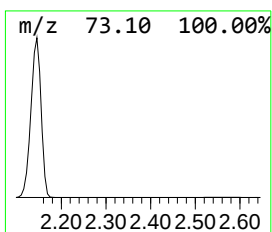
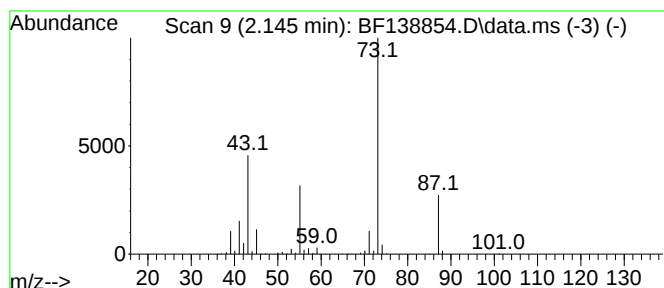
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.145	201.58 ng	2745040	1,4-Dichlorobenzene-d4	6.839

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	23
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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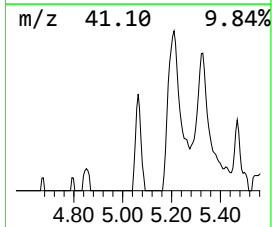
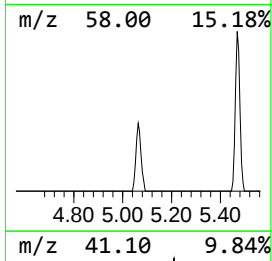
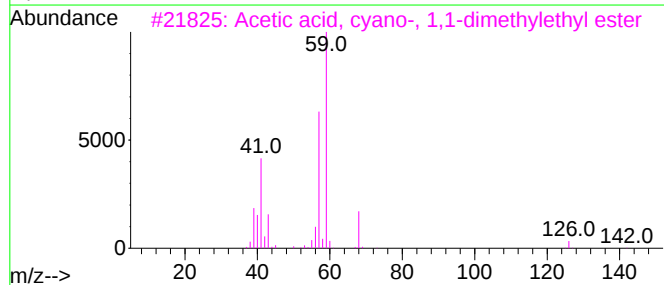
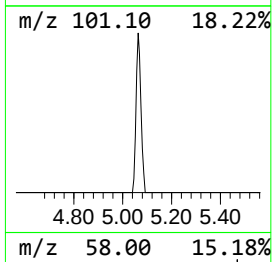
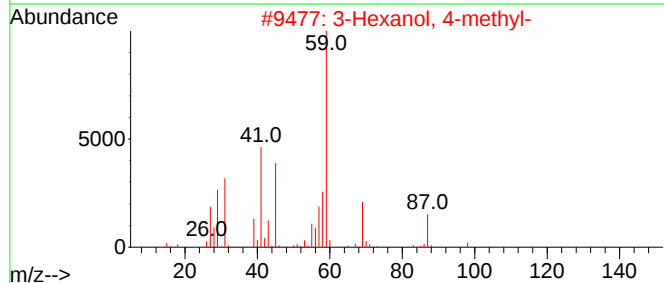
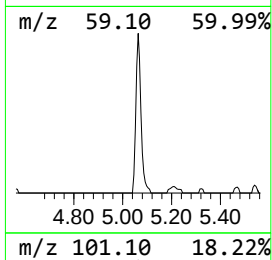
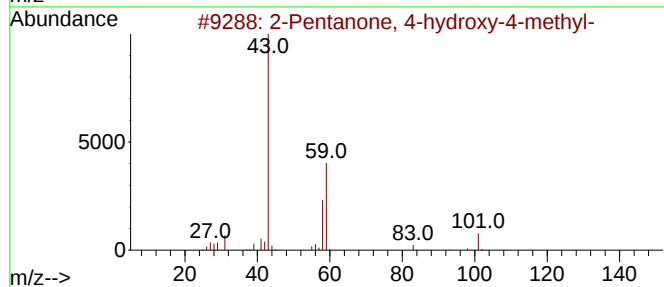
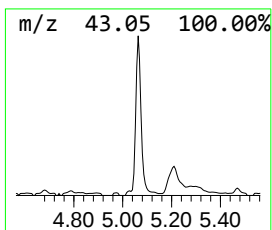
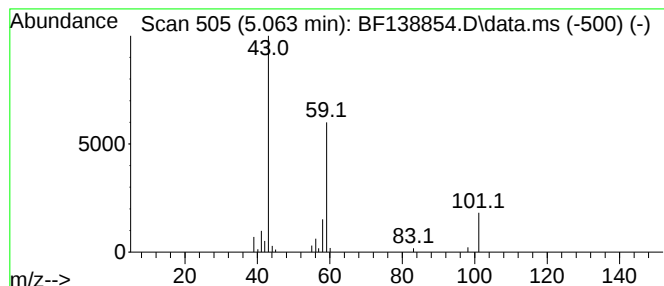
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	3.22 ng	43870	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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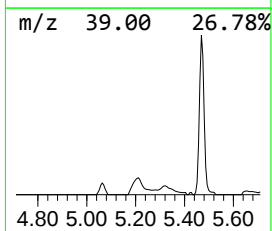
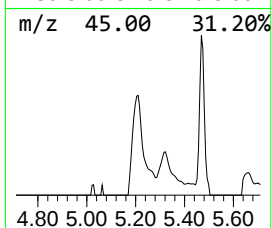
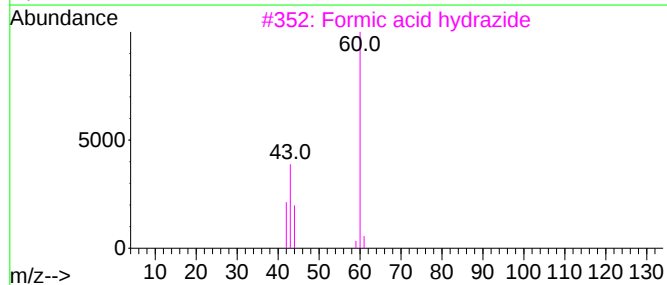
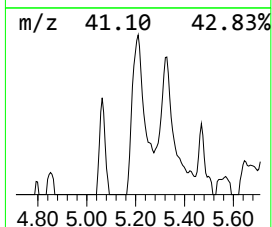
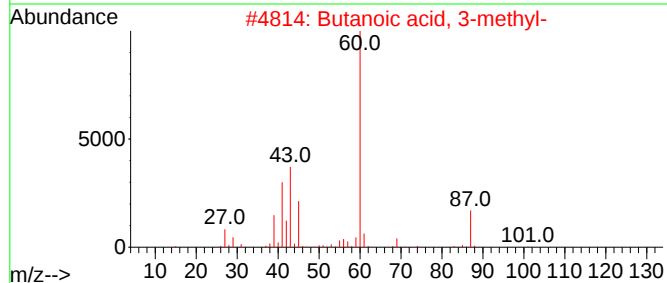
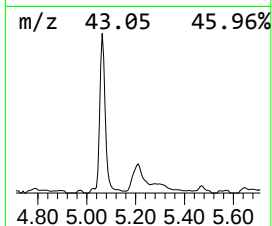
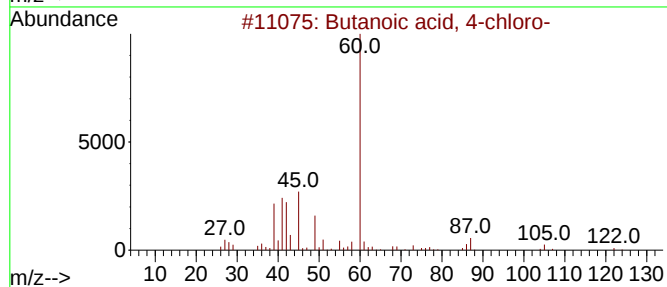
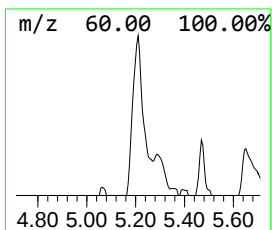
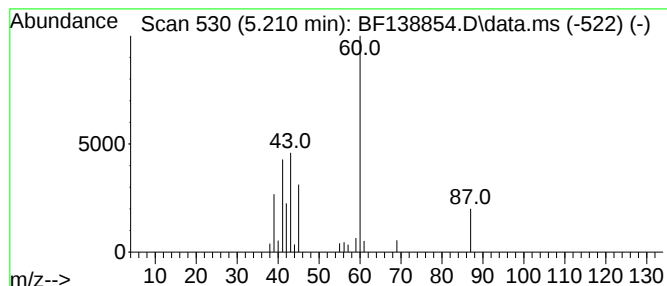
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Peak Number 4 Butanoic acid, 4-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	3.63 ng	49408	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	72
2			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
3			Formic acid hydrazide	60	CH4N2O	000624-84-0	50
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5			1-Hexanamine	101	C6H15N	000111-26-2	9



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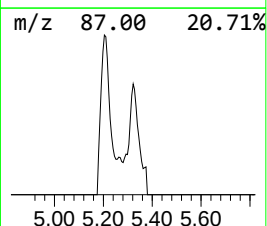
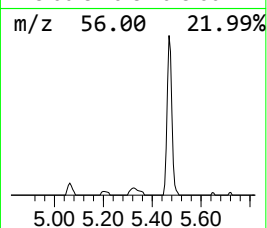
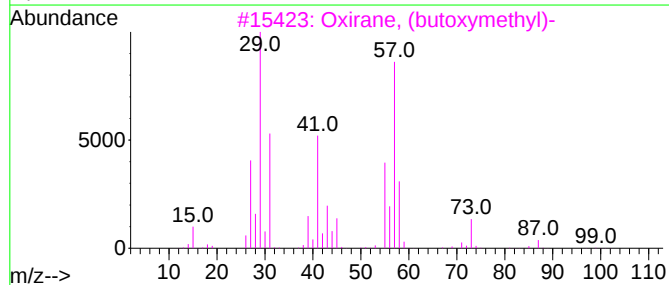
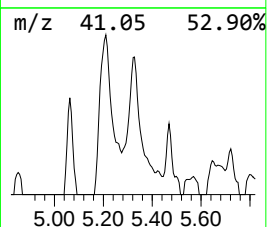
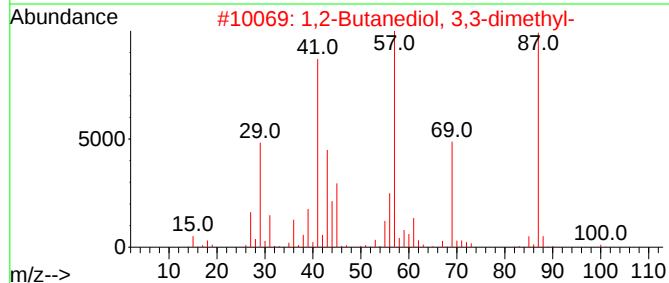
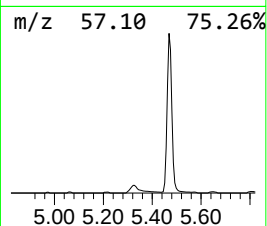
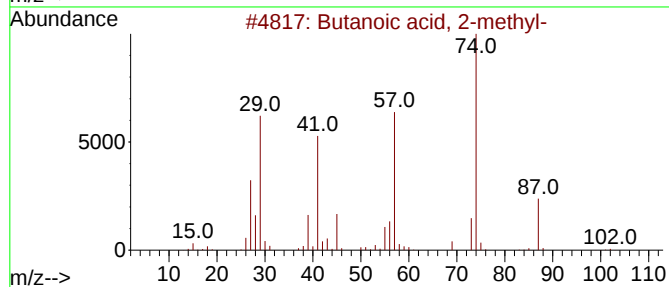
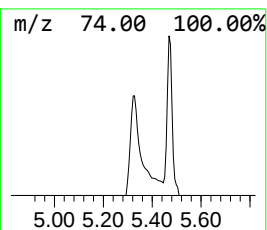
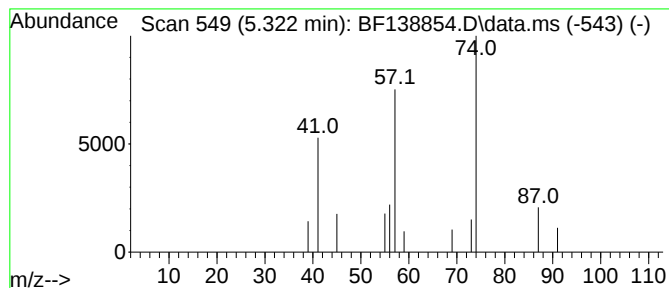
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Butanoic acid, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.322	2.11 ng	28690	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	64
2			1,2-Butanediol, 3,3-dimethyl-	118	C6H14O2	059562-82-2	22
3			Oxirane, (butoxymethyl)-	130	C7H14O2	002426-08-6	9
4			Methyl-2-O-methyl.alpha.d-glucop...	208	C8H16O6	015064-82-1	9
5			1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	9



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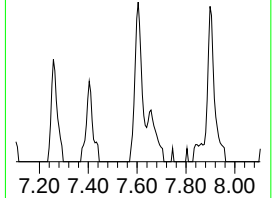
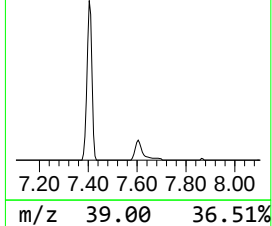
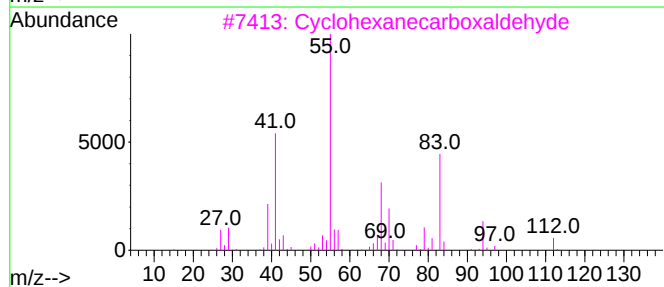
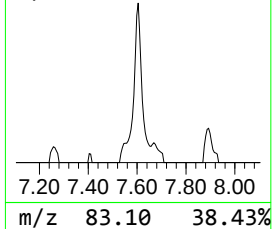
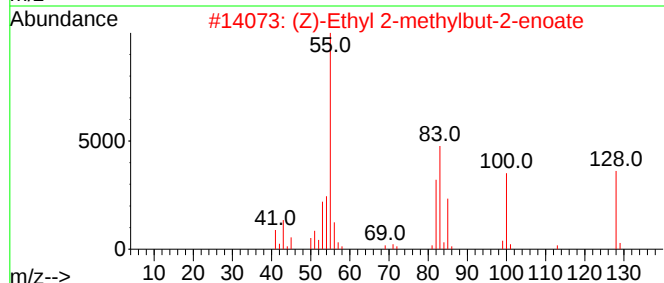
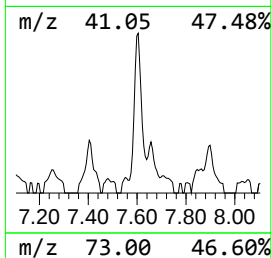
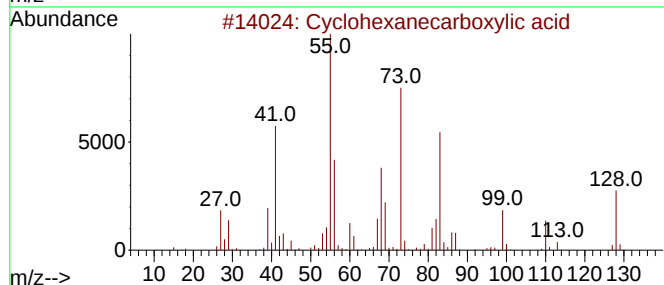
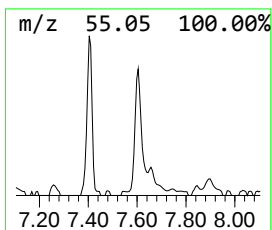
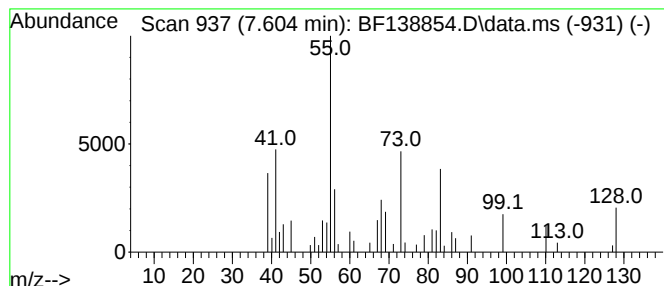
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Cyclohexanecarboxylic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.604	3.03 ng	55144	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	97
2			(Z)-Ethyl 2-methylbut-2-enoate	128	C7H12O2	016509-44-7	35
3			Cyclohexanecarboxaldehyde	112	C7H12O	002043-61-0	23
4			3,7-Decadiene, 2,9-dimethyl-	166	C12H22	074630-13-0	17
5			Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	16



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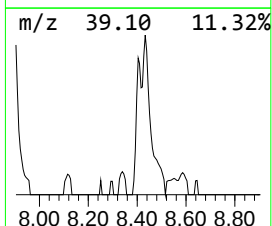
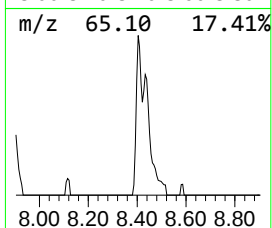
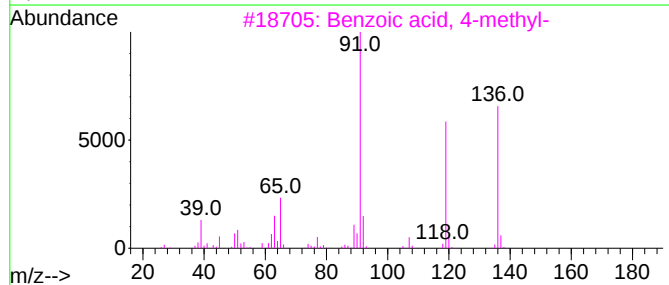
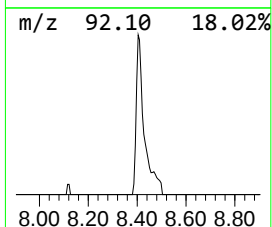
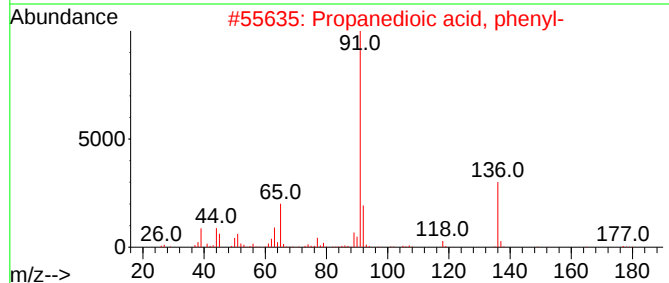
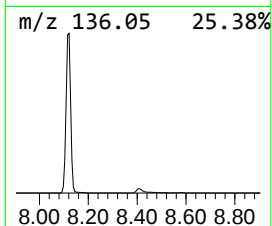
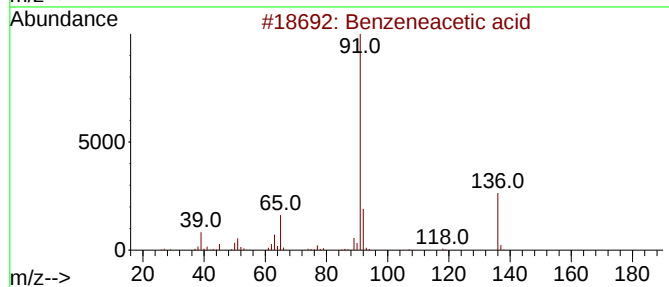
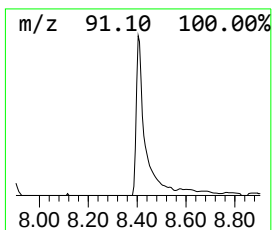
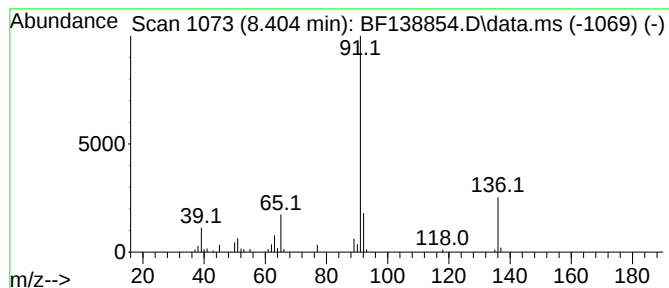
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzeneacetic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.404	2.78 ng	50652	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	93
2			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	86
3			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	64
4			Benzene, (iodomethyl)-	218	C7H7I	000620-05-3	47
5			Bicyclo[3.2.0]hepta-2,6-diene, 5...	126	C7H7Cl	023610-81-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138854.D
Acq On : 07 Aug 2024 21:08
Operator : RC/JU
Sample : P3430-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
925-K1-WP0-0-0.25-073124

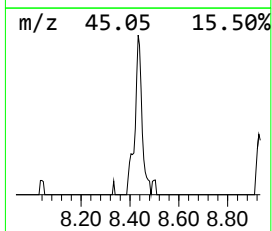
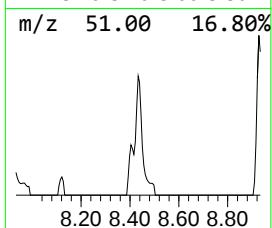
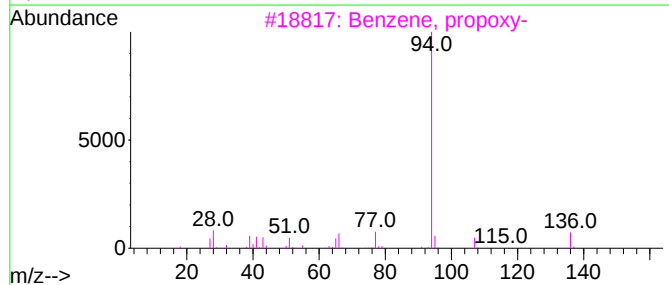
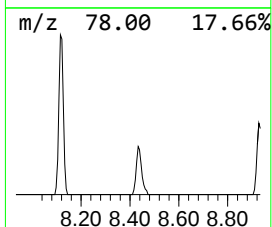
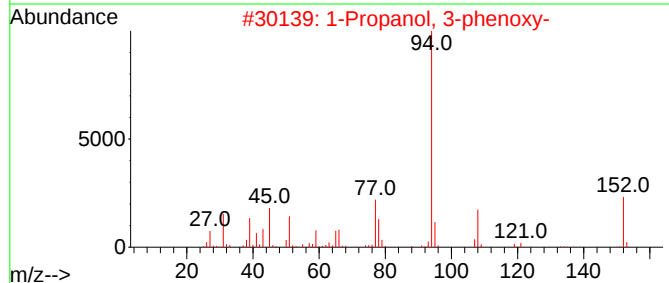
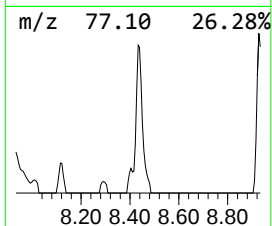
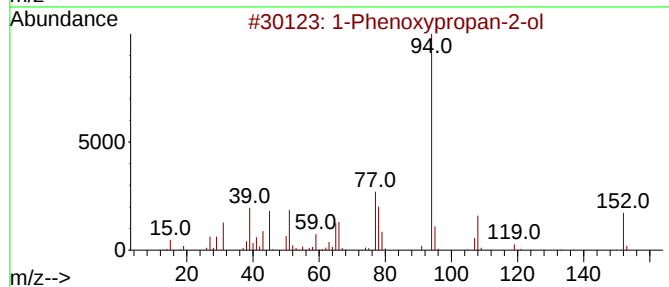
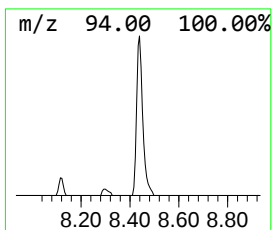
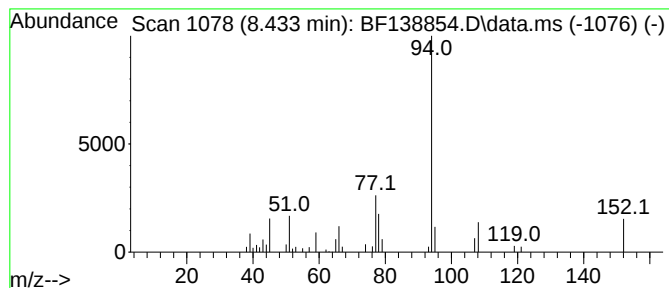
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	4.15 ng	75418	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3			Benzene, propoxy-	136	C9H12O	000622-85-5	50
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	45
5			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138854.D
Acq On : 07 Aug 2024 21:08
Operator : RC/JU
Sample : P3430-05
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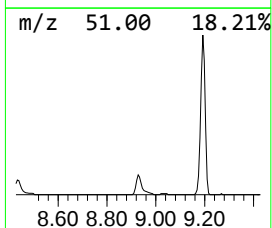
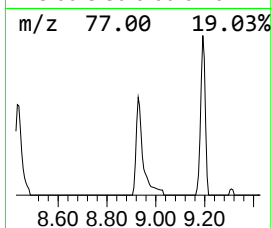
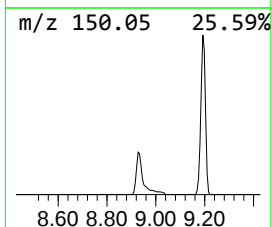
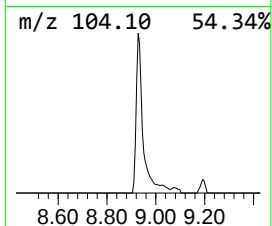
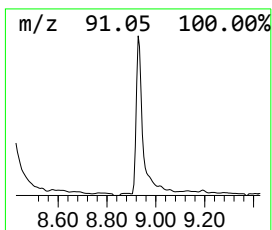
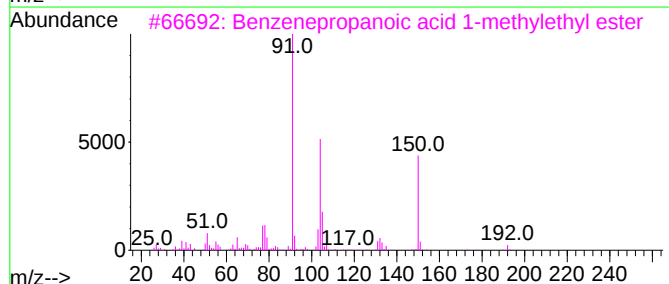
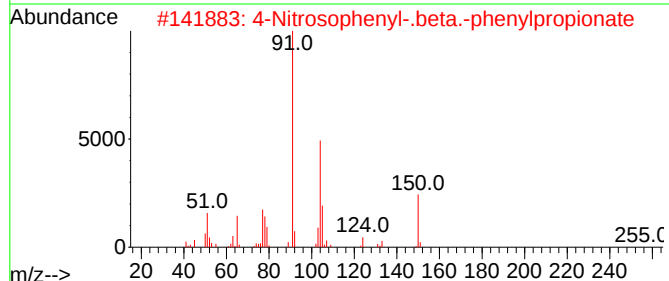
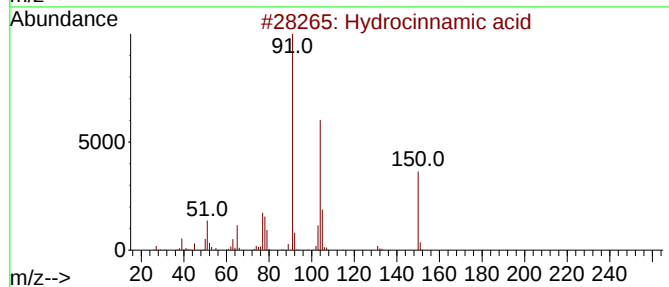
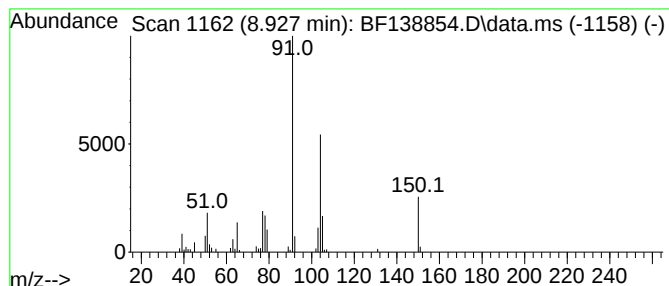
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hydrocinnamic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.927	5.61 ng	102072	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrocinnamic acid	150	C9H10O2	000501-52-0	95
2			4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	91
3			Benzenepropanoic acid 1-methylet...	192	C12H16O2	022767-95-9	64
4			.beta.-Phenylethyl butyrate	192	C12H16O2	000103-52-6	53
5			Acetic acid, trifluoro-, 2-pheny...	218	C10H9F3O2	055419-66-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138854.D
Acq On : 07 Aug 2024 21:08
Operator : RC/JU
Sample : P3430-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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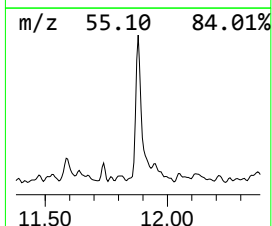
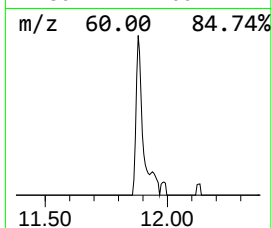
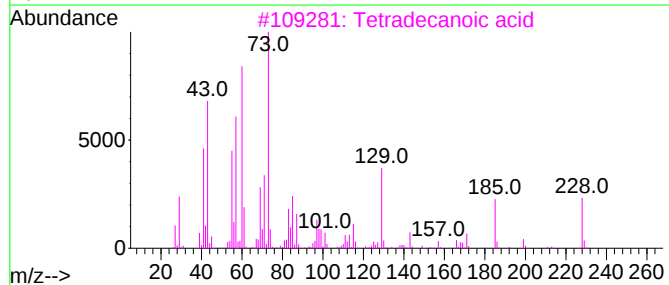
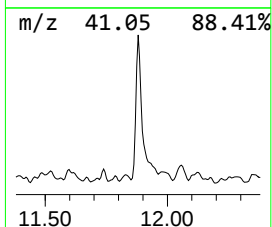
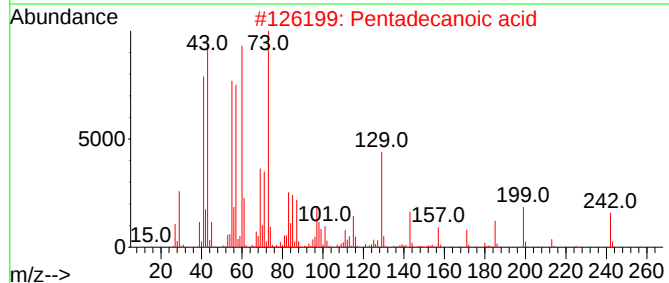
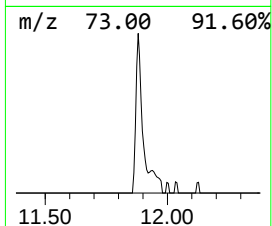
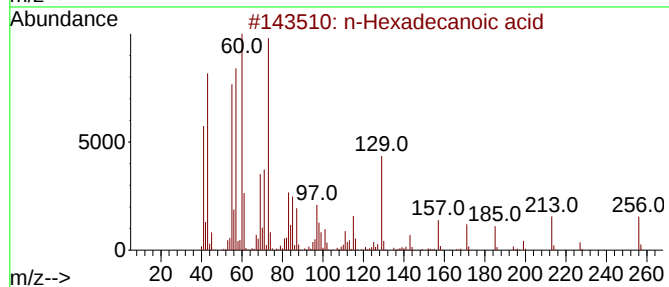
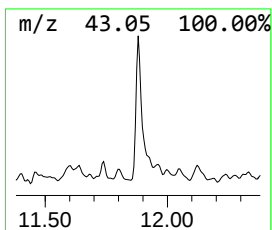
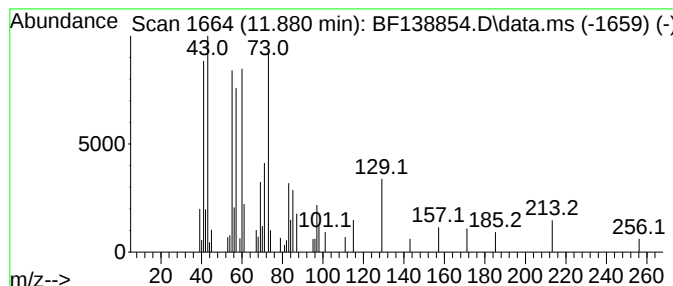
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	2.85 ng	54037	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138854.D
Acq On : 07 Aug 2024 21:08
Operator : RC/JU
Sample : P3430-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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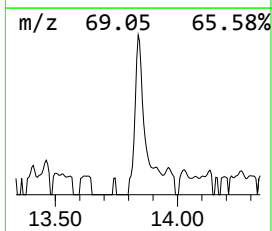
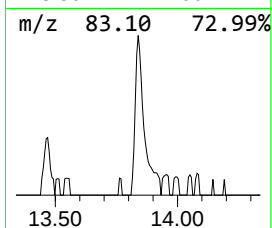
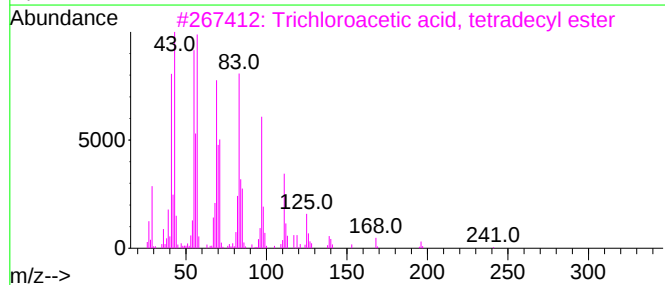
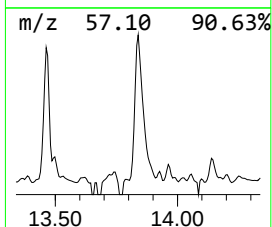
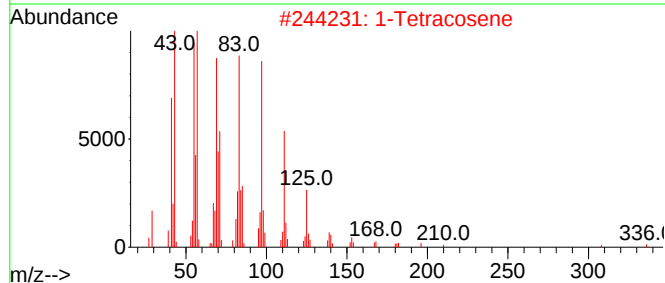
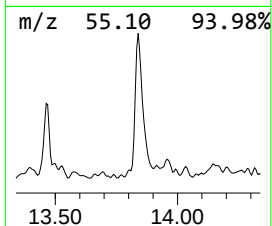
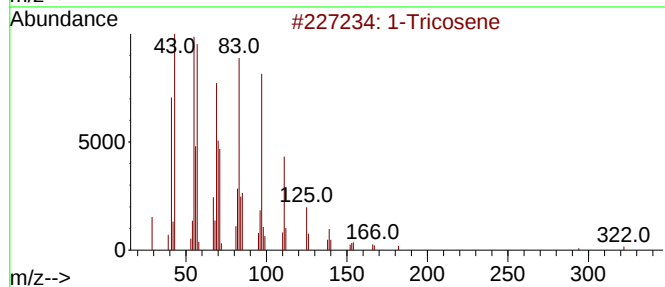
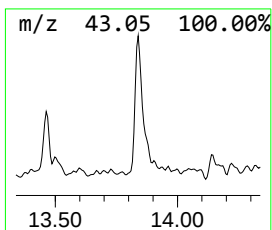
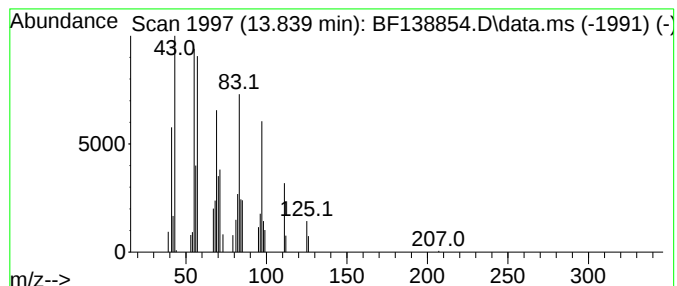
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Tricosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	4.85 ng	47152	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene			322	C23H46	018835-32-0	95
2	1-Tetracosene			336	C24H48	010192-32-2	91
3	Trichloroacetic acid, tetradecyl...			358	C16H29Cl3O2	074339-52-9	91
4	1-Heneicosanol			312	C21H44O	015594-90-8	91
5	1-Docosene			308	C22H44	001599-67-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138854.D
Acq On : 07 Aug 2024 21:08
Operator : RC/JU
Sample : P3430-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
925-K1-WP0-0-0.25-073124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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
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2-Pentanone, 4-...	5.063	3.2	ng	43870	1	6.839	272357	20.0
Butanoic acid, ...	5.210	3.6	ng	49408	1	6.839	272357	20.0
Butanoic acid, ...	5.322	2.1	ng	28690	1	6.839	272357	20.0
Cyclohexanecarb...	7.604	3.0	ng	55144	2	8.122	363867	20.0
Benzeneacetic acid	8.404	2.8	ng	50652	2	8.122	363867	20.0
1-Phenoxypropan...	8.433	4.2	ng	75418	2	8.122	363867	20.0
Hydrocinnamic acid	8.927	5.6	ng	102072	2	8.122	363867	20.0
n-Hexadecanoic ...	11.880	2.9	ng	54037	4	11.357	378585	20.0
1-Tricosene	13.839	4.8	ng	47152	5	13.998	194490	20.0