

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
 Data File : BF134472.D
 Acq On : 25 Jul 2023 20:18
 Operator : CG\JU
 Sample : 03668-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 332

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-BF072423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134472.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	13	rVB	390980	474850	19.59%	2.723%
2	3.593	251	256	266	rBV	23873	42017	1.73%	0.241%
3	4.457	398	403	422	rBV	861945	992920	40.97%	5.693%
4	5.075	503	508	521	rBV	993024	1181754	48.76%	6.776%
5	5.475	572	576	591	rBV	1240816	1325043	54.68%	7.598%
6	6.475	742	746	767	rBV	2015932	2029606	83.75%	11.638%
7	6.669	774	779	789	rBV	31081	54168	2.24%	0.311%
8	6.834	803	807	815	rBV	736426	616084	25.42%	3.533%
9	7.398	899	903	906	rBV	1689548	1406884	58.05%	8.067%
10	8.110	1021	1024	1027	rBV	877544	675772	27.89%	3.875%
11	9.187	1203	1207	1210	rBV	2892370	2423376	100.00%	13.896%
12	9.310	1223	1228	1239	rVB	1798130	1749003	72.17%	10.029%
13	9.869	1319	1323	1326	rBV	825791	661822	27.31%	3.795%
14	10.663	1455	1458	1466	rBV	78760	75150	3.10%	0.431%
15	10.839	1484	1488	1496	rBV2	15417	30173	1.25%	0.173%
16	10.939	1503	1505	1512	rVB	21541	33352	1.38%	0.191%
17	11.363	1573	1577	1580	rBV	752473	611932	25.25%	3.509%
18	12.463	1761	1764	1770	rVB3	85329	86393	3.56%	0.495%
19	12.586	1782	1785	1787	rBV	53720	47998	1.98%	0.275%
20	12.610	1787	1789	1792	rVB	77875	54744	2.26%	0.314%
21	12.816	1822	1824	1829	rVB2	135121	126935	5.24%	0.728%
22	12.957	1844	1848	1852	rBV	2104860	1854002	76.50%	10.631%
23	13.180	1883	1886	1895	rVB5	32717	56035	2.31%	0.321%
24	13.527	1942	1945	1951	rBV2	22247	29442	1.21%	0.169%
25	13.880	1999	2005	2012	rVB6	61013	134505	5.55%	0.771%
26	14.022	2025	2029	2033	rBV	363122	375760	15.51%	2.155%
27	15.527	2281	2285	2296	rVB	210370	290028	11.97%	1.663%

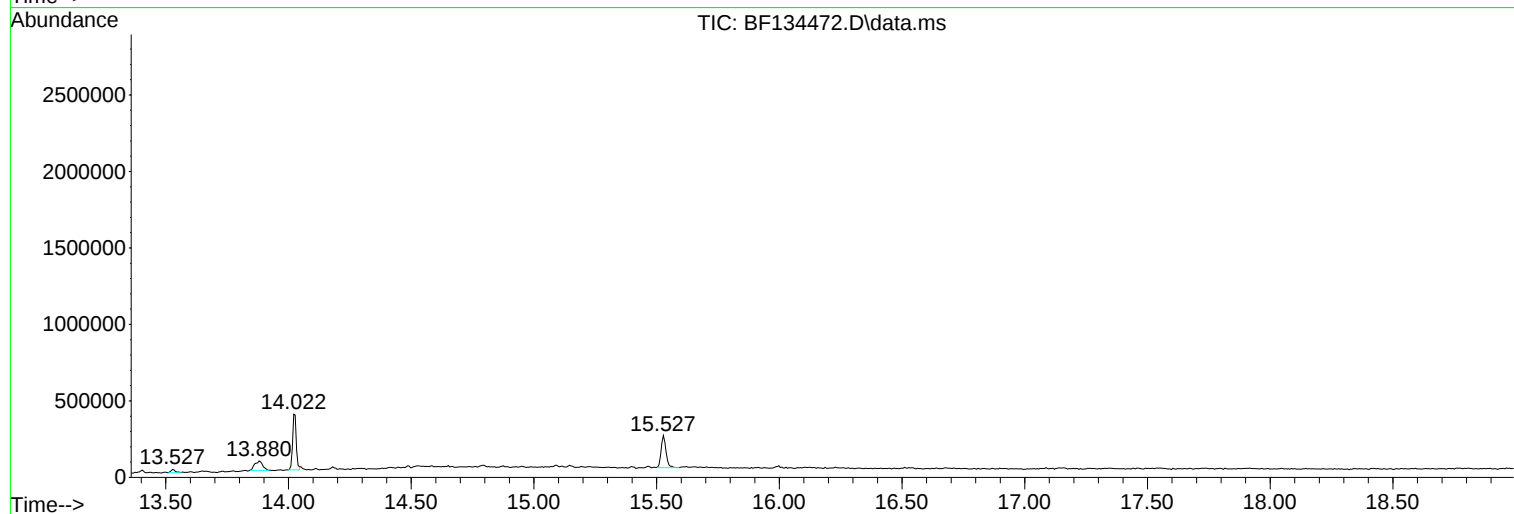
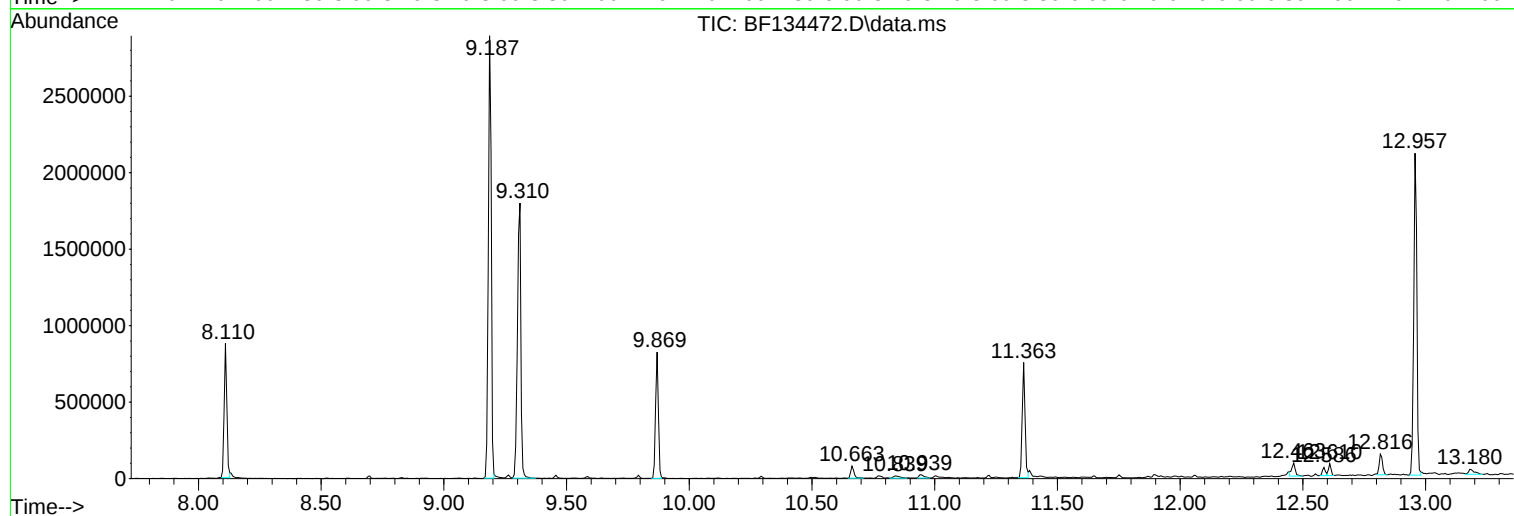
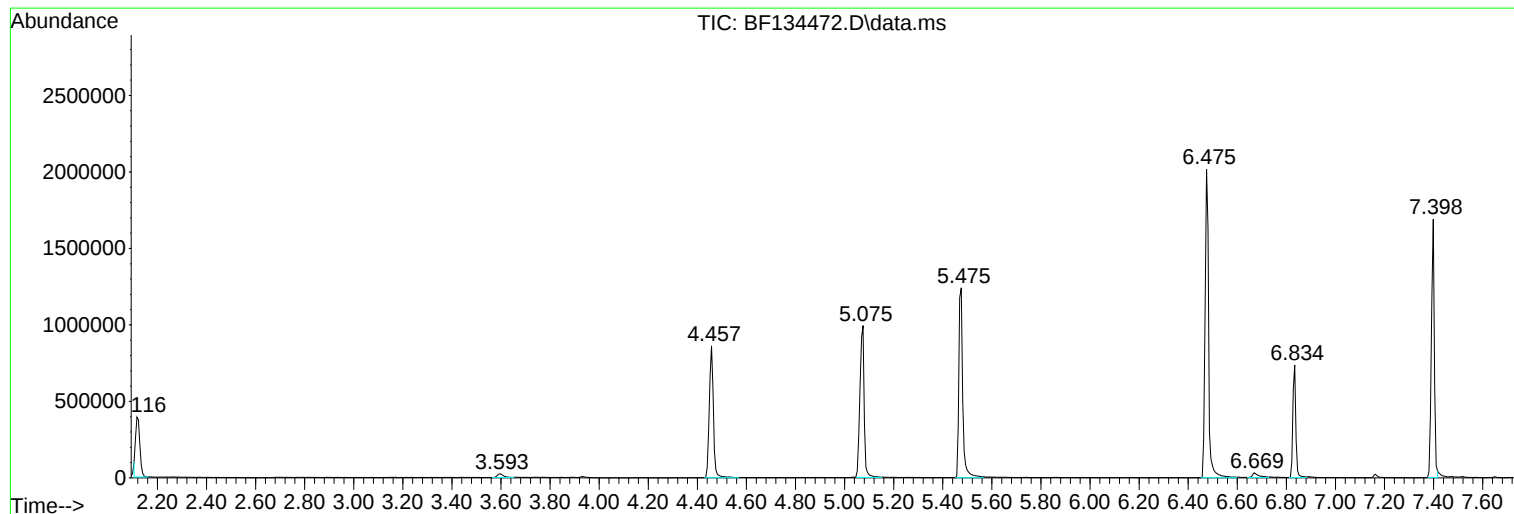
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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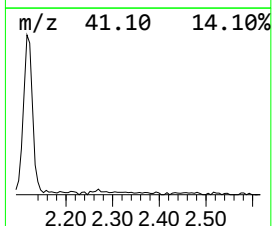
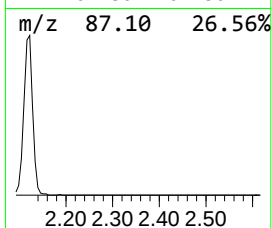
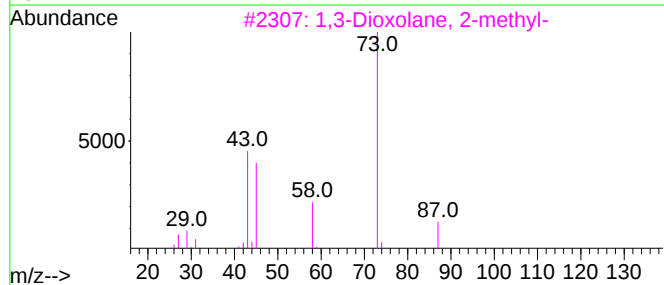
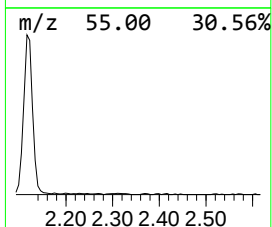
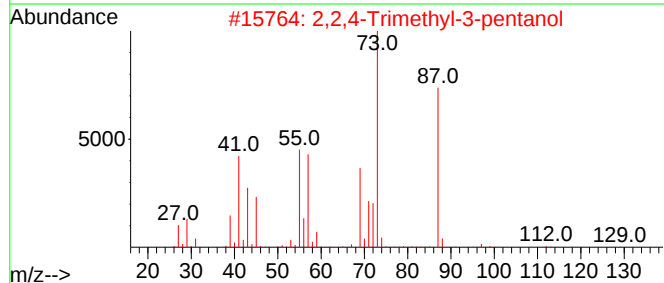
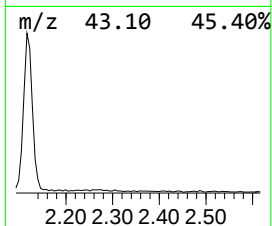
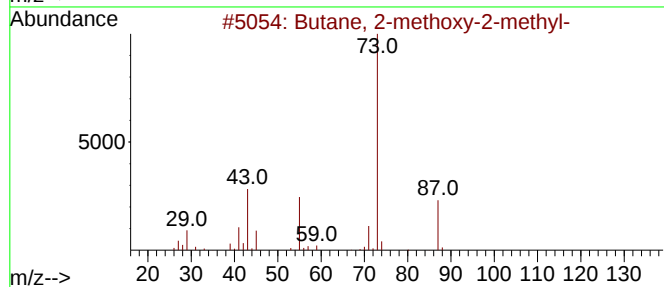
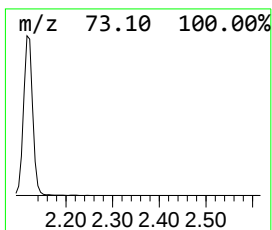
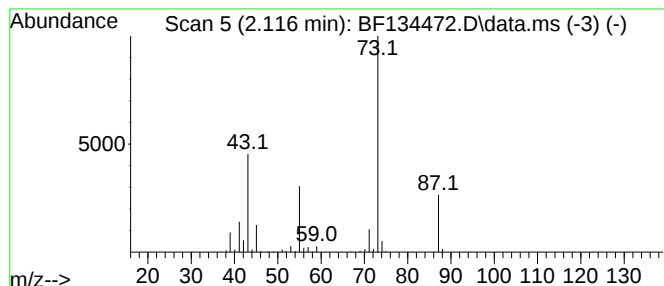
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	15.42 ng	474850	1,4-Dichlorobenzene-d4	6.834

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	32
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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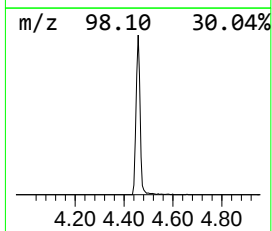
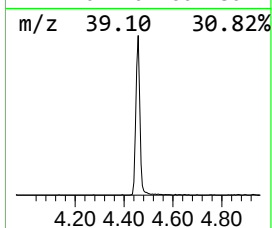
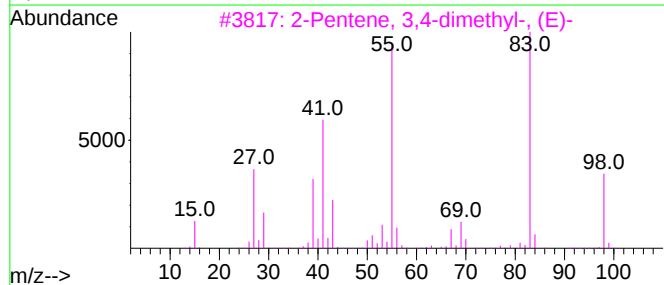
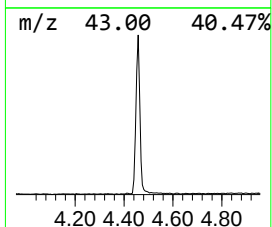
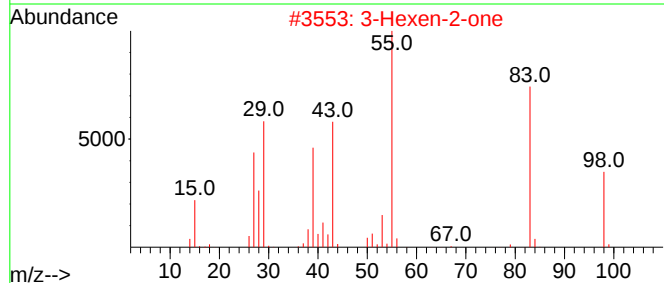
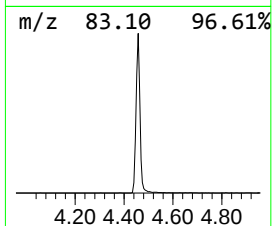
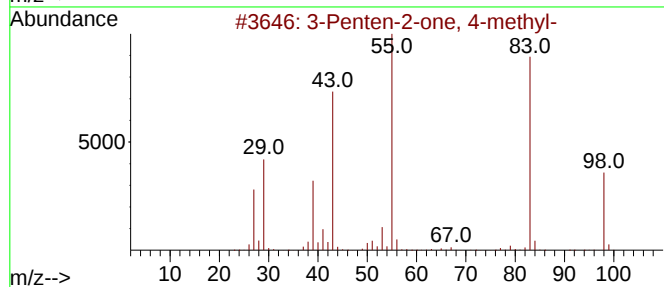
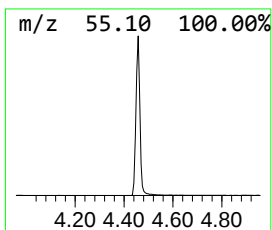
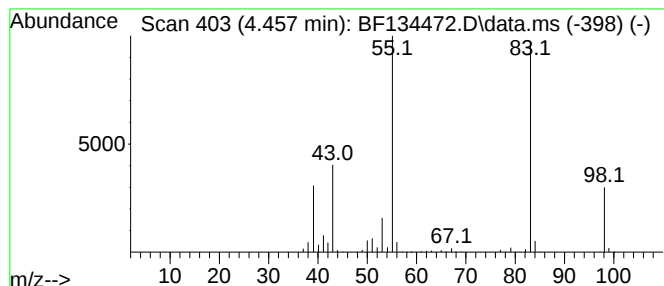
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	32.23 ng	992920	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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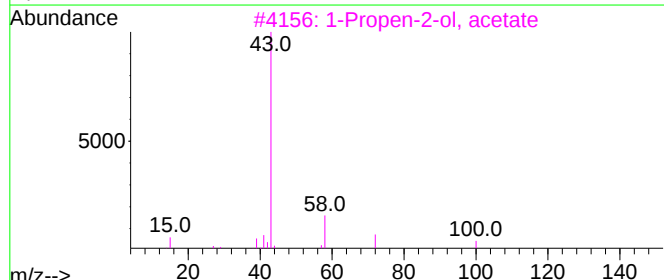
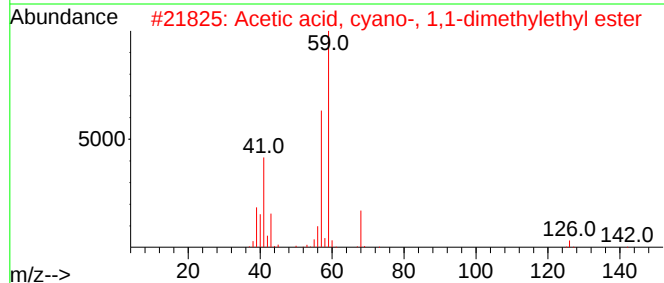
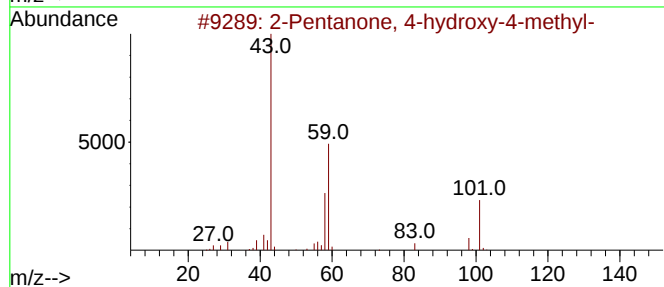
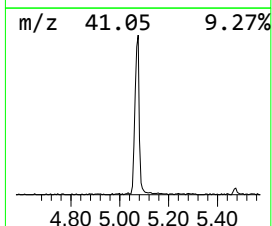
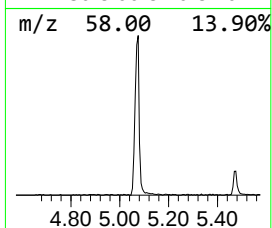
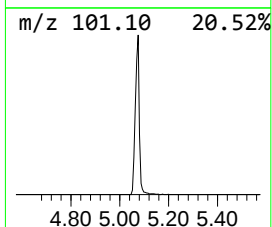
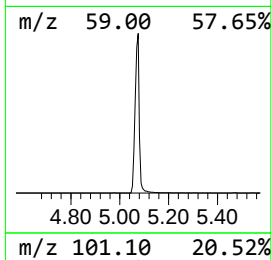
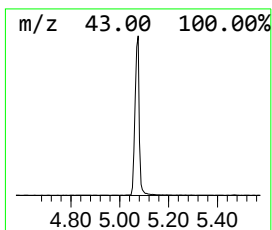
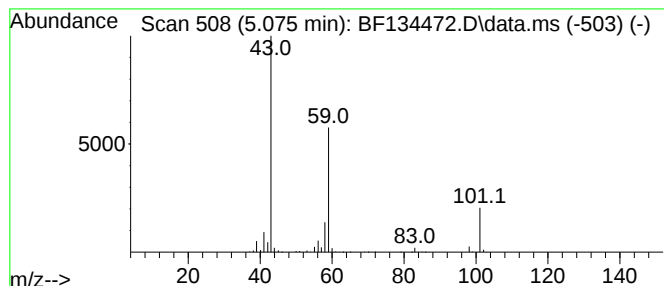
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	38.36 ng	1181750	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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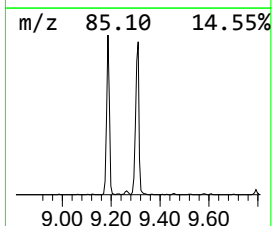
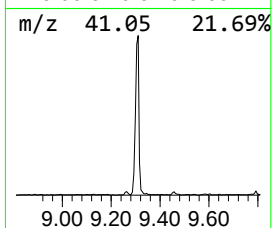
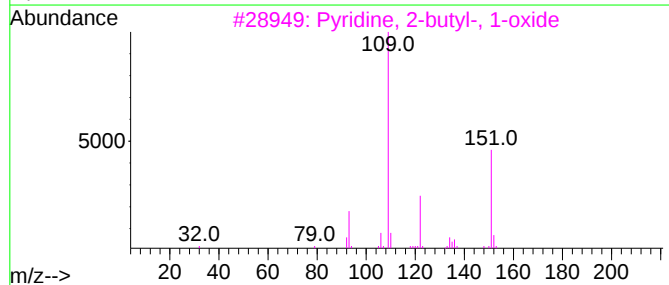
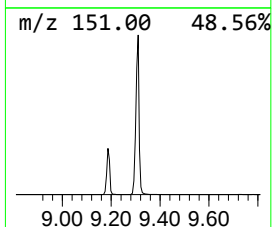
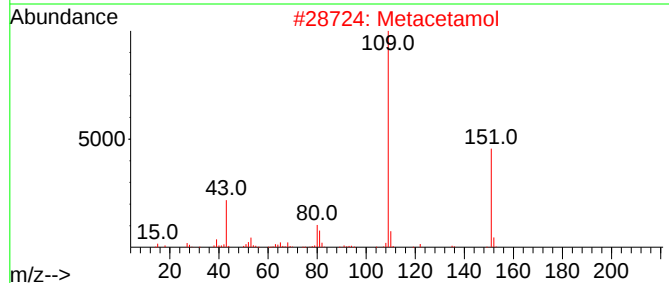
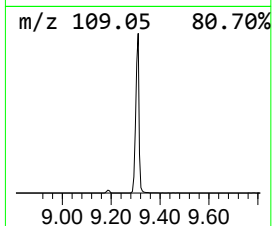
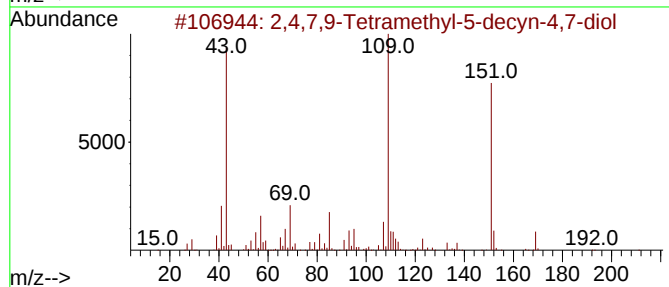
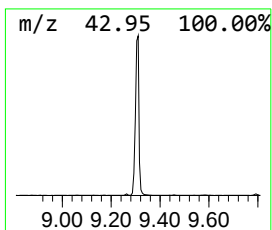
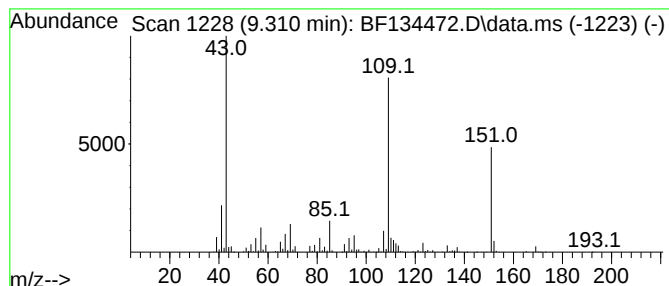
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Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.310	52.85 ng	1749000	Acenaphthene-d10			9.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	91
2	Metacetamol	151	C8H9NO2		000621-42-1	59
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	59
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2		001006-96-8	59
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3		1000107-08-7	59



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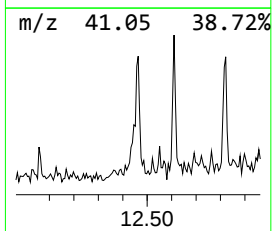
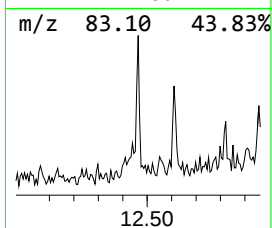
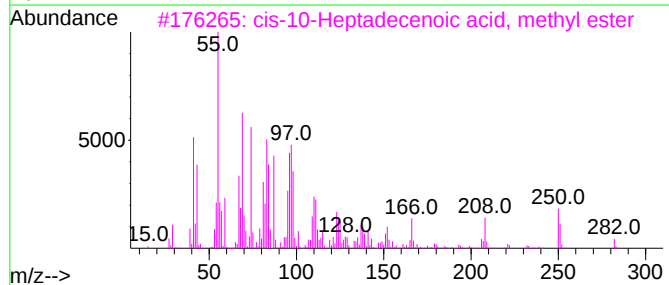
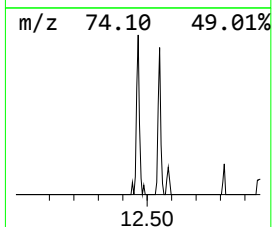
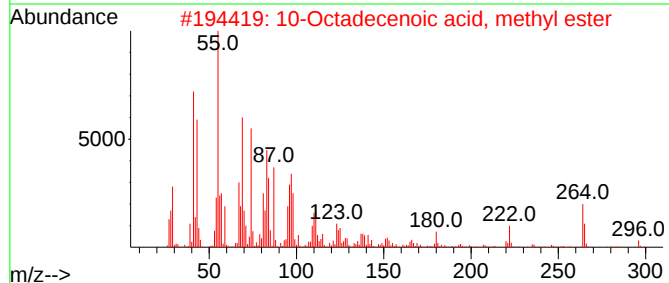
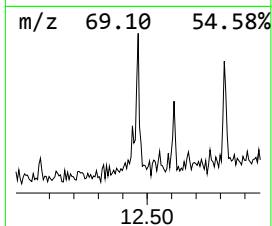
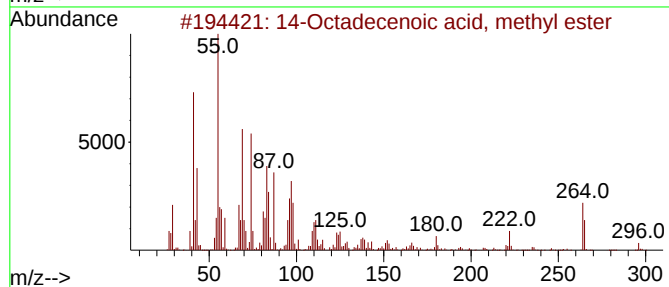
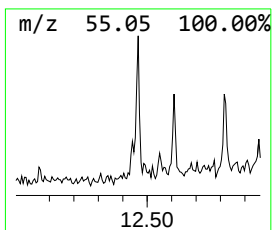
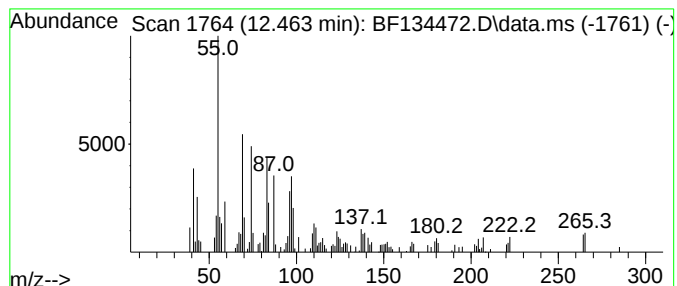
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Peak Number 5 14-Octadecenoic acid, methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	2.82 ng	86393	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90
2			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	86
3			cis-10-Heptadecenoic acid, methyl ester	282	C18H34O2	1000333-62-1	78
4			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	78
5			Cyclopropanoic acid, 2-hexyl ester	282	C18H34O2	010152-61-1	74



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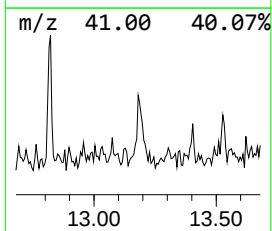
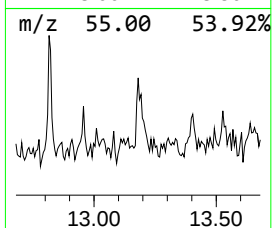
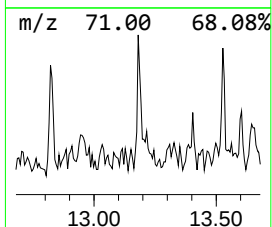
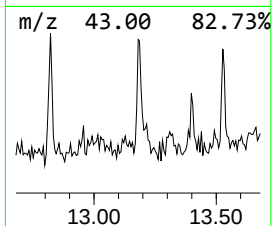
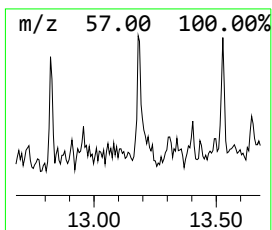
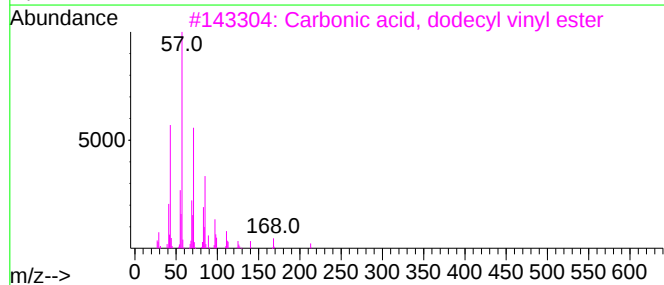
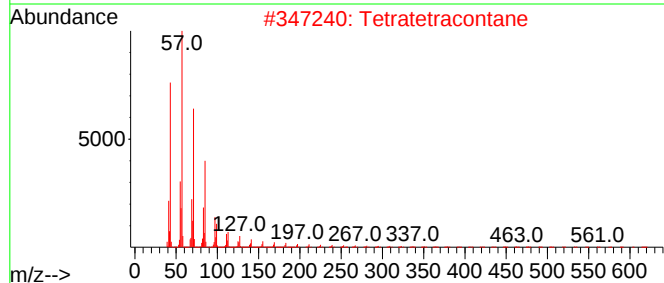
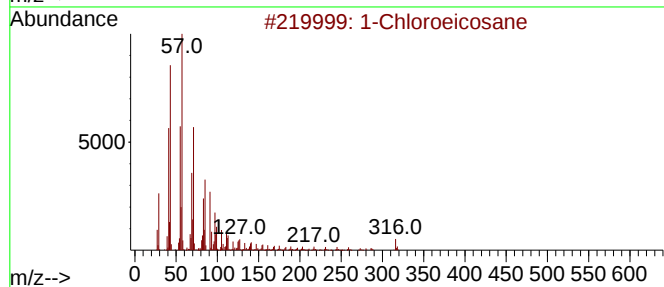
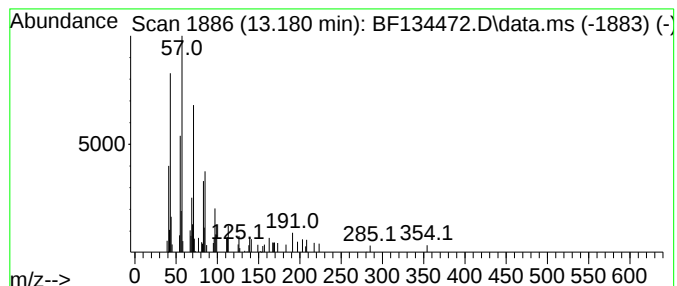
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Chloroeicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.180	2.98 ng	56035	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Chloroeicosane	316	C20H41Cl	042217-02-7	80
2			Tetratetracontane	619	C44H90	007098-22-8	64
3			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	58
4			Cyclohexanone, 4-(1,1-dimethylpr...	168	C11H20O	016587-71-6	50
5			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134472.D
Acq On : 25 Jul 2023 20:18
Operator : CG\JU
Sample : 03668-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
332

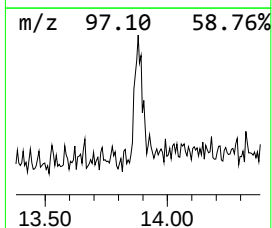
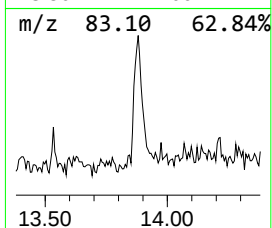
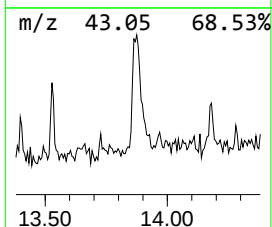
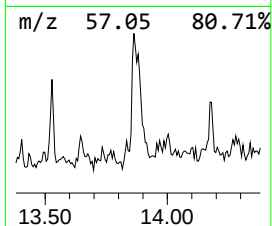
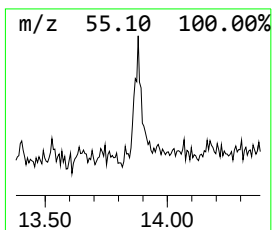
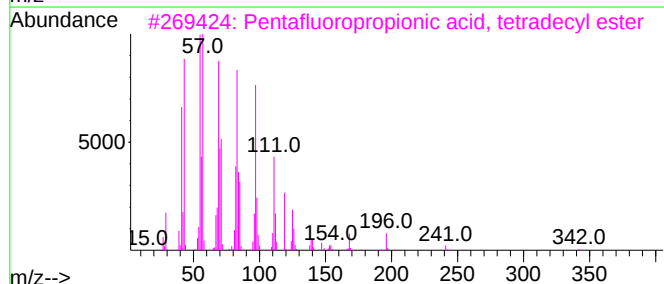
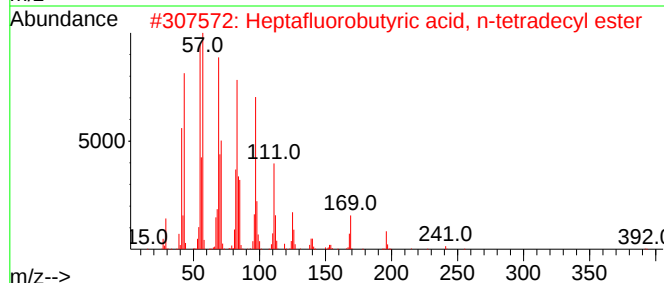
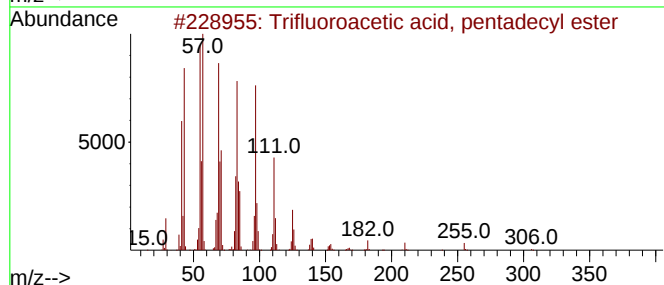
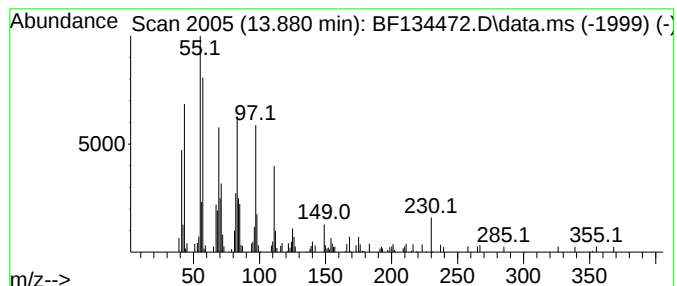
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	7.16 ng	134505	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
2			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	76
3			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	76
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	72
5			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134472.D
Acq On : 25 Jul 2023 20:18
Operator : CG\JU
Sample : 03668-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
332

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.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
Butane, 2-metho...	2.116	15.4	ng	474850	1	6.834	616084	20.0
3-Penten-2-one,...	4.457	32.2	ng	992920	1	6.834	616084	20.0
2-Pentanone, 4-...	5.075	38.4	ng	1181750	1	6.834	616084	20.0
2,4,7,9-Tetrame...	9.310	52.9	ng	1749000	3	9.869	661822	20.0
14-Octadecenoic...	12.463	2.8	ng	86393	4	11.363	611932	20.0
1-Chloroeicosane	13.180	3.0	ng	56035	5	14.027	375760	20.0
Trifluoroacetic...	13.880	7.2	ng	134505	5	14.027	375760	20.0