

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120424\
 Data File : BF140739.D
 Acq On : 04 Dec 2024 20:49
 Operator : RC/JU
 Sample : P5072-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-738

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-BF112124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140739.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	4	11	24	rVB	757706	1183543	46.03%	7.251%
2	2.269	24	30	39	rVB	32546	54469	2.12%	0.334%
3	5.099	505	511	533	rVB	134263	215817	8.39%	1.322%
4	5.504	574	580	602	rBV	1402960	1892185	73.59%	11.592%
5	6.510	745	751	778	rBV	1375362	2007841	78.09%	12.300%
6	6.869	807	812	818	rBV	327007	402728	15.66%	2.467%
7	7.434	902	908	930	rBV	977348	1312534	51.05%	8.041%
8	7.687	946	951	964	rBV	31412	57934	2.25%	0.355%
9	8.151	1024	1030	1048	rVB	386010	532654	20.72%	3.263%
10	9.222	1206	1212	1222	rBV	2000198	2571283	100.00%	15.752%
11	9.904	1323	1328	1341	rBV	463203	594219	23.11%	3.640%
12	10.616	1444	1449	1458	rBV	140063	186796	7.26%	1.144%
13	10.698	1458	1463	1479	rBV	1075402	1452823	56.50%	8.900%
14	11.398	1576	1582	1590	rBV	430590	581097	22.60%	3.560%
15	12.616	1785	1789	1795	rBV	20428	26472	1.03%	0.162%
16	12.845	1824	1828	1835	rVB	22896	34658	1.35%	0.212%
17	12.986	1846	1852	1857	rBV	1470856	1965800	76.45%	12.043%
18	13.463	1925	1933	1943	rBV	337418	517301	20.12%	3.169%
19	14.045	2028	2032	2041	rVB	269295	391979	15.24%	2.401%
20	15.545	2282	2287	2297	rBV	200457	341175	13.27%	2.090%

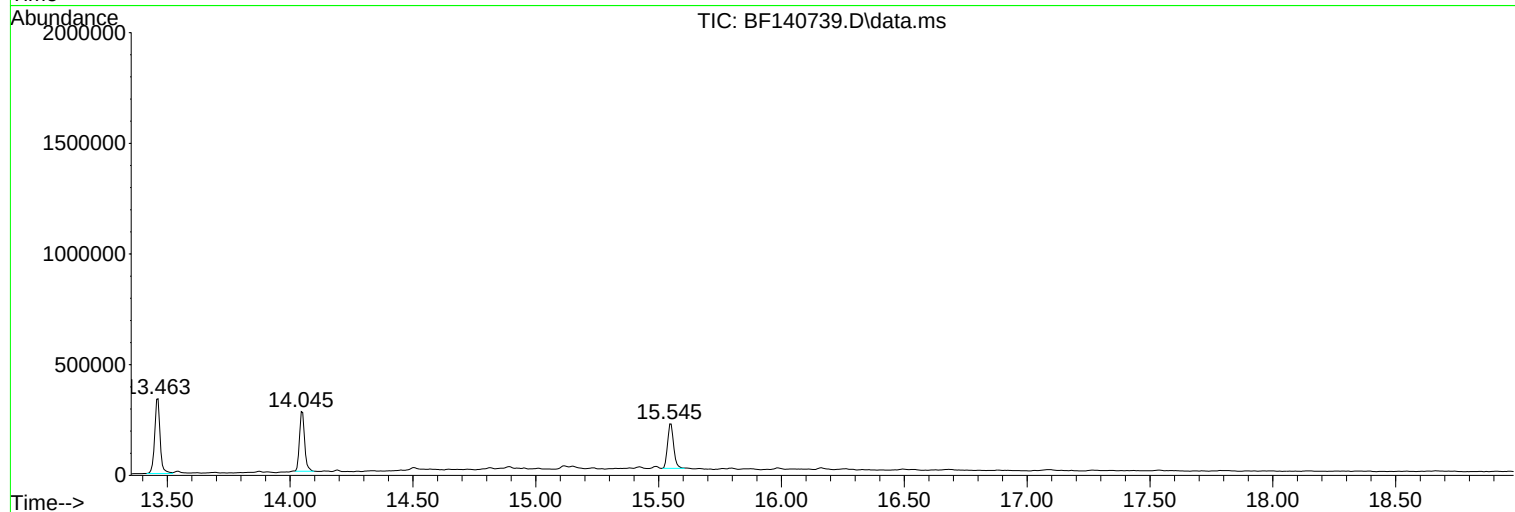
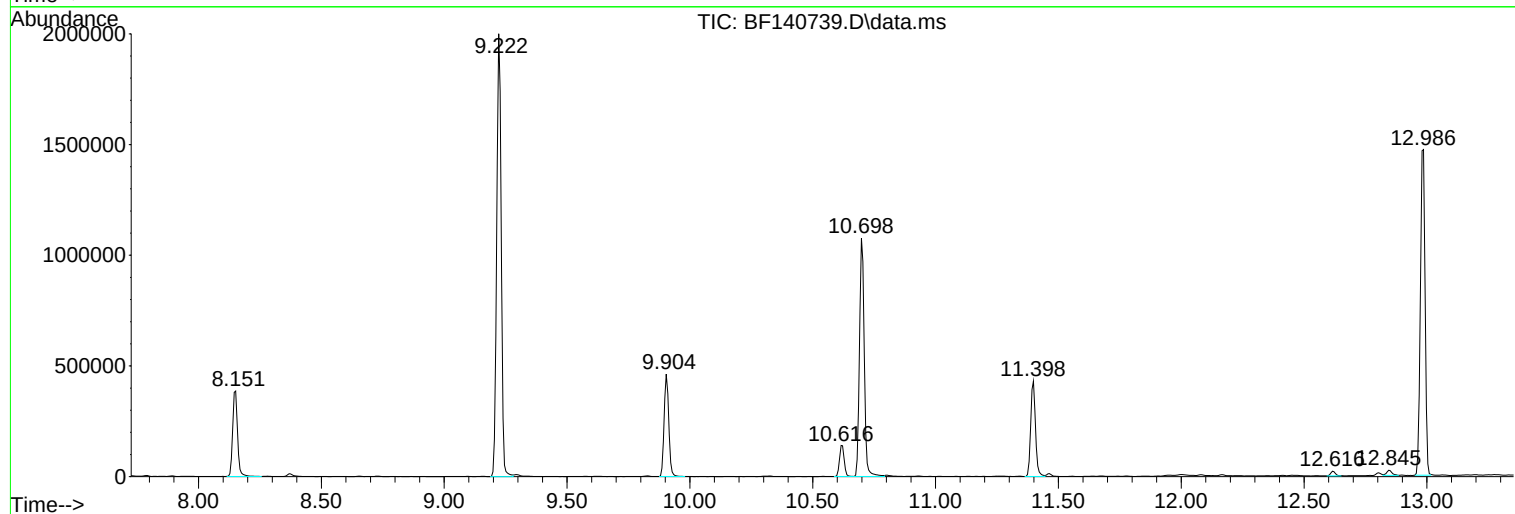
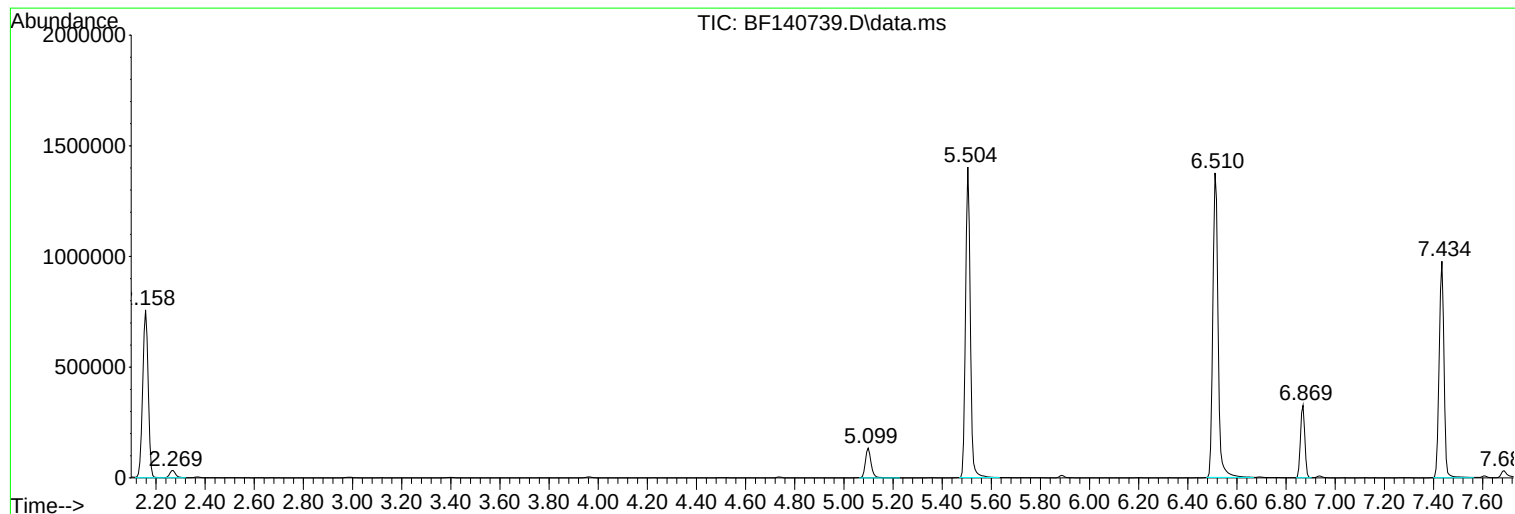
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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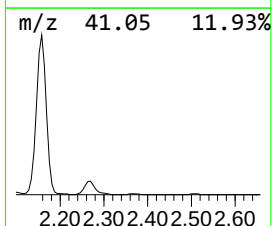
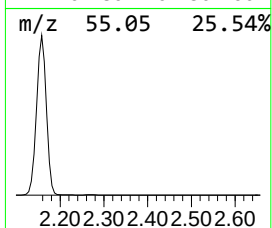
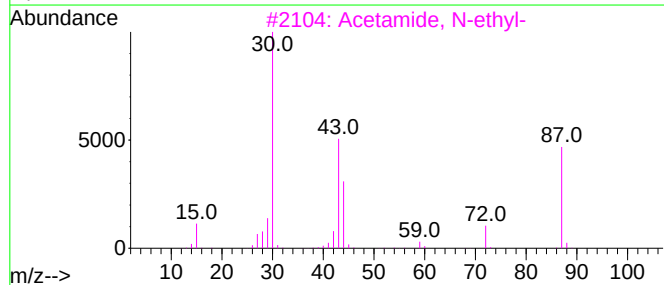
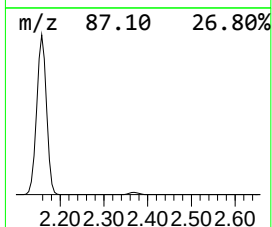
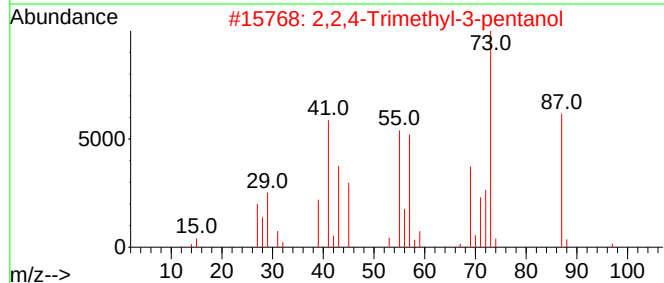
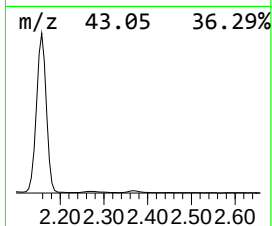
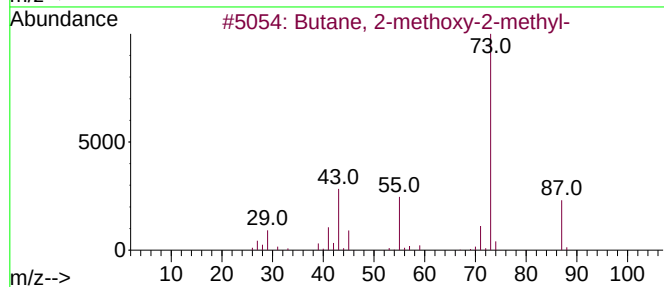
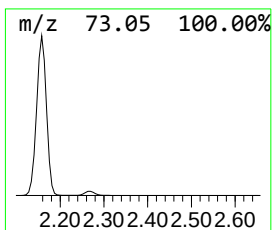
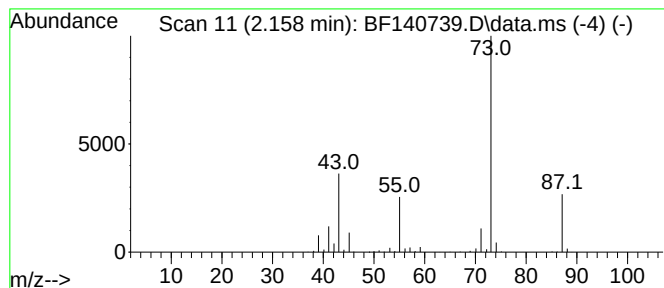
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.158	58.78 ng	1183540	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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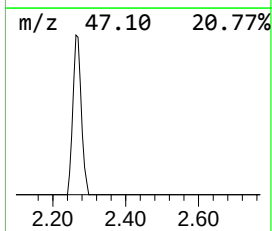
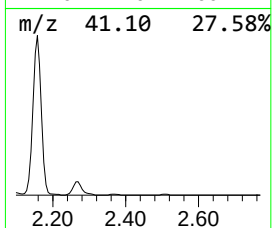
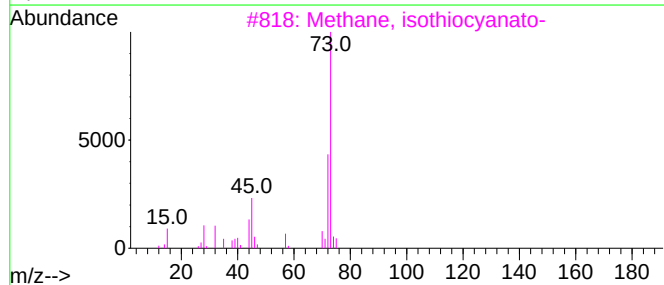
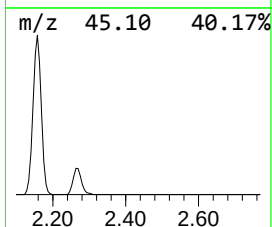
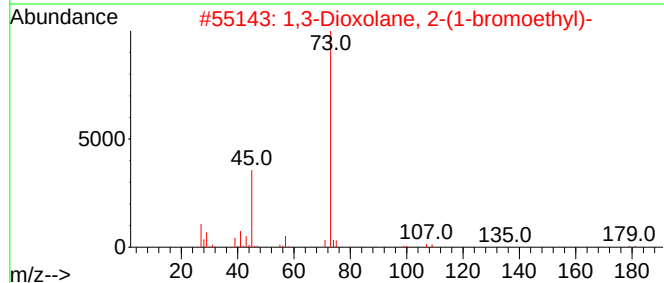
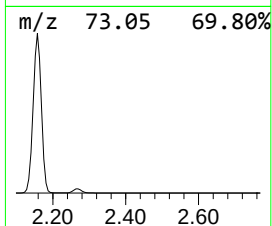
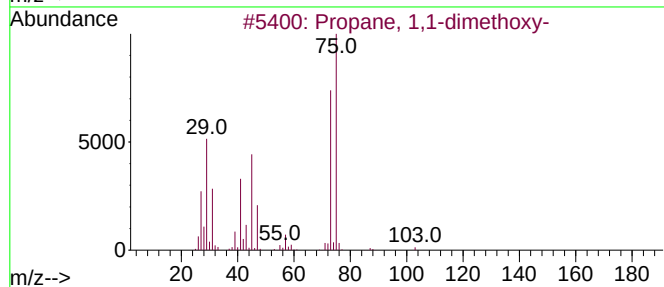
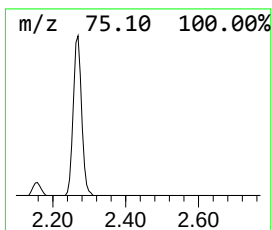
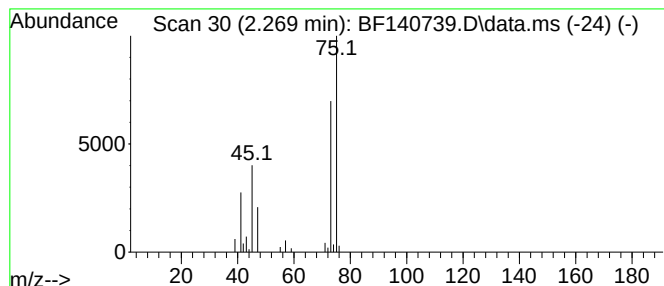
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	2.71 ng	54469	1,4-Dichlorobenzene-d4	6.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	27
3		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9



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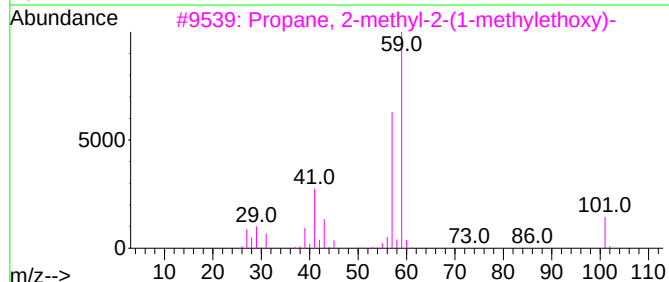
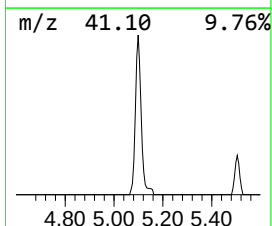
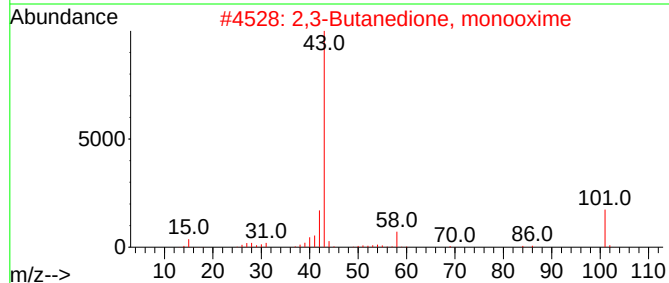
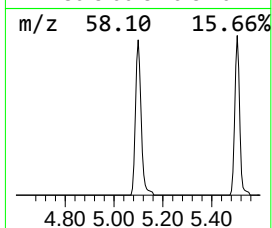
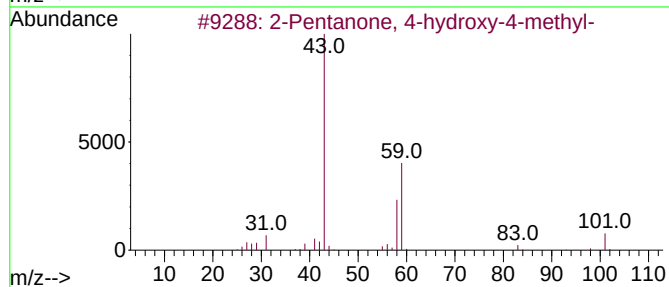
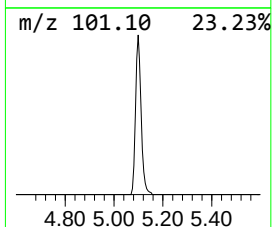
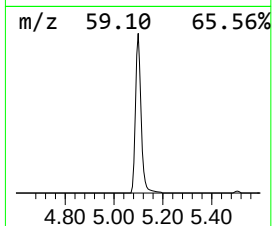
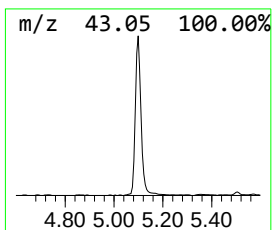
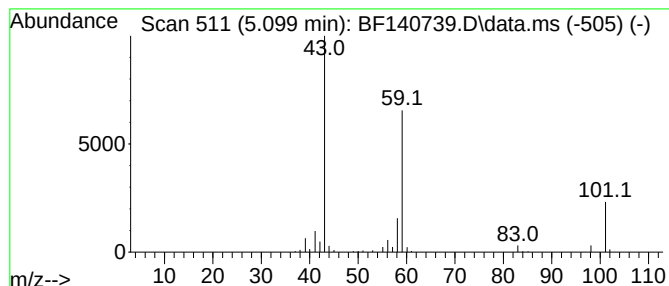
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.099	10.72 ng	215817	1,4-Dichlorobenzene-d4			6.869
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	35
3	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	23
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10



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Instrument :
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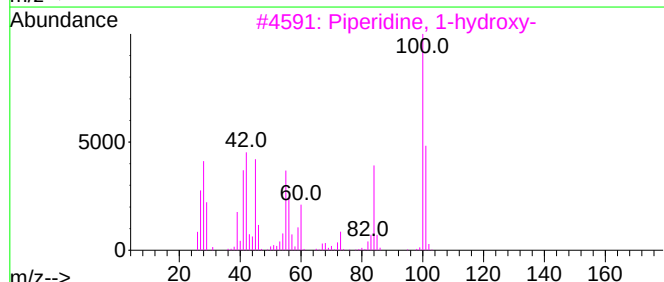
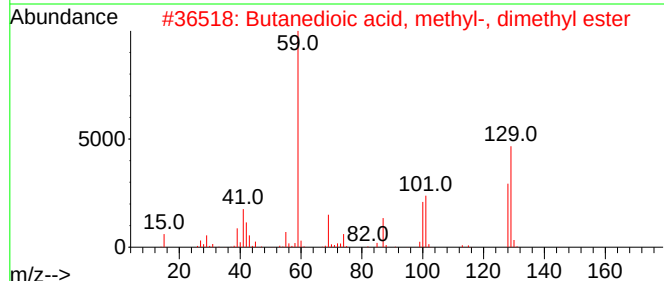
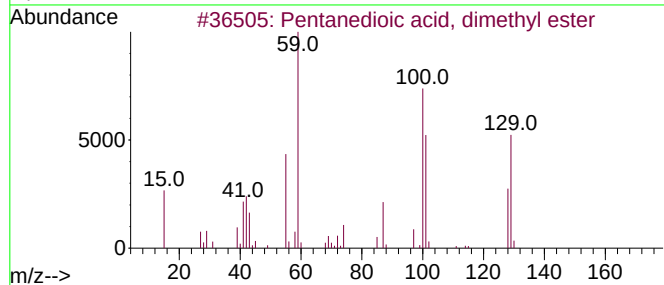
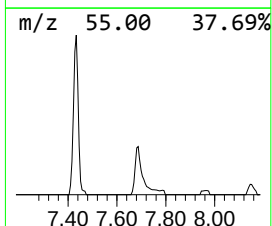
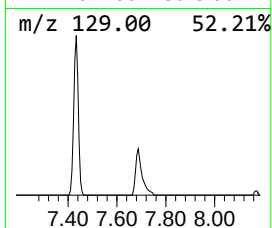
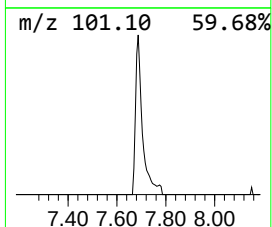
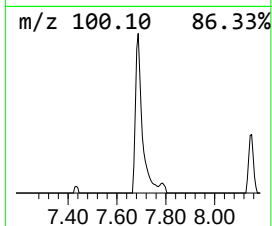
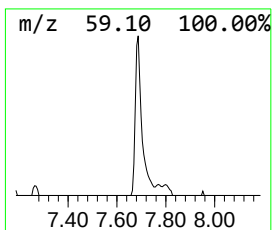
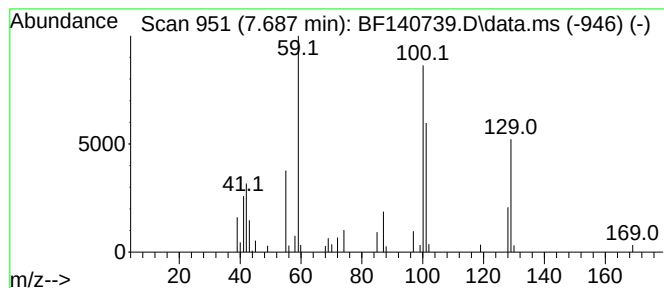
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Peak Number 4 Pentanedioic acid, dimethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.687	2.18 ng	57934	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	83
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	40
3			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	35
4			3-Methyl-2-butenic acid, heptad...	338	C22H42O2	1000282-89-9	25
5			Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	16



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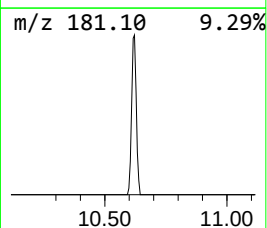
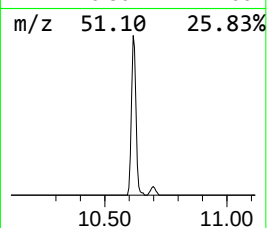
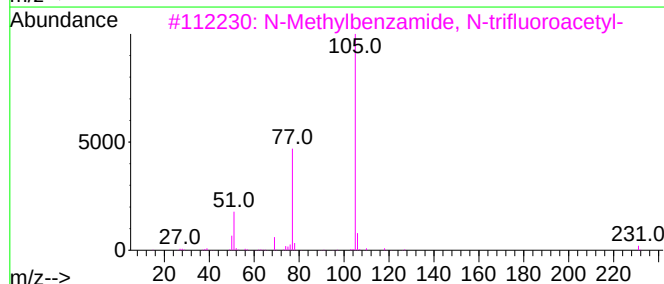
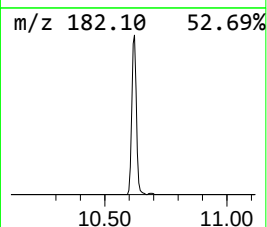
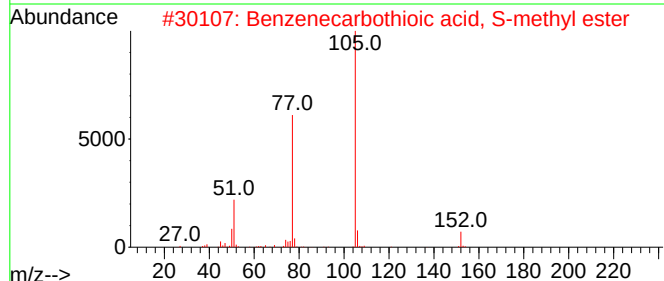
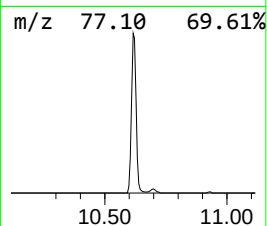
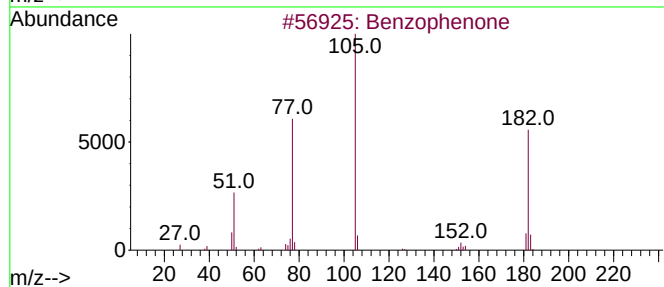
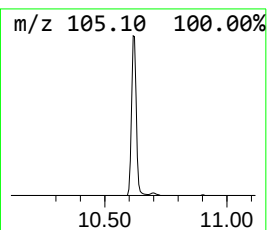
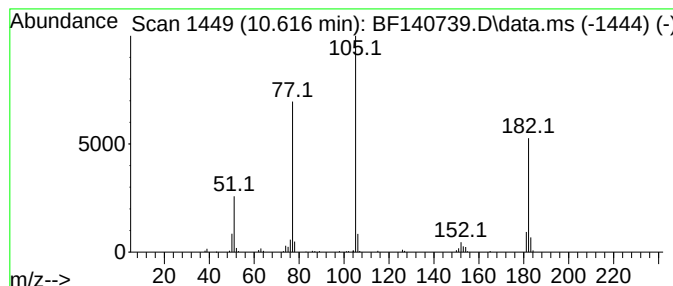
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	6.29 ng	186796	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4			.beta.-Benzilmonoxime	225	C14H11NO2	014090-77-8	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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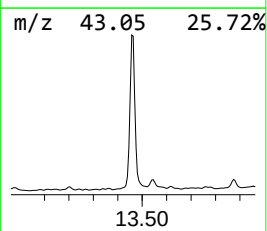
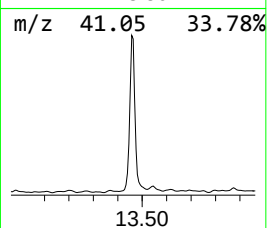
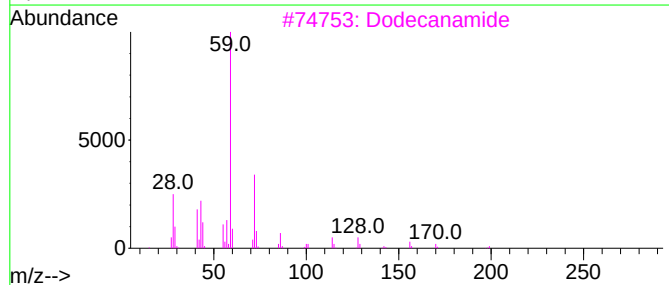
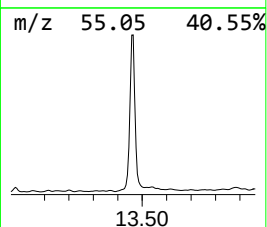
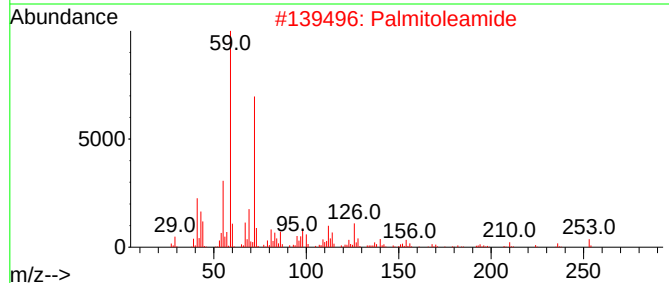
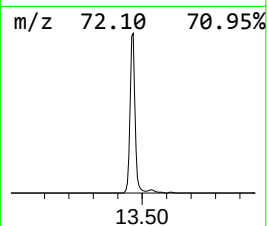
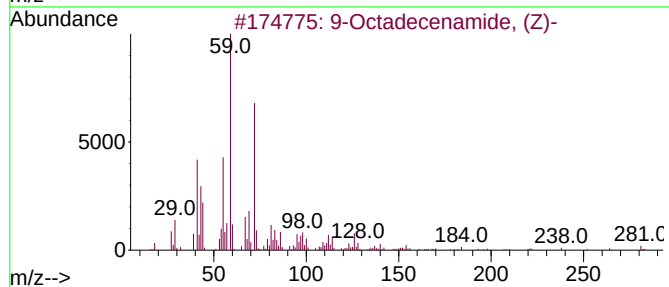
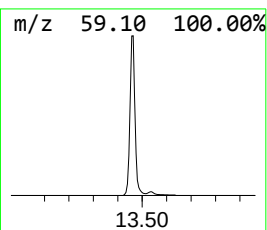
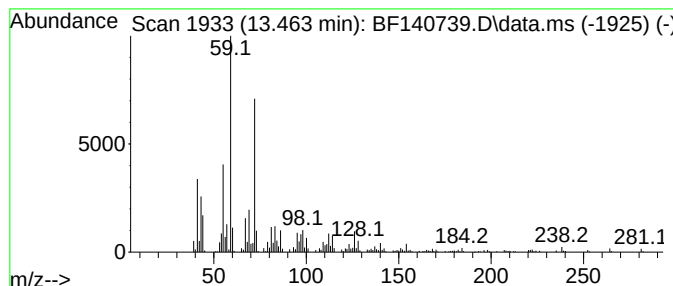
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	26.39 ng	517301	Chrysene-d12	14.051

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		Palmitoleamide	253	C16H31NO	106010-22-4	80
3		Dodecanamide	199	C12H25NO	001120-16-7	59
4		Octanamide	143	C8H17NO	000629-01-6	59
5		4-Ethyl-3-octanol	158	C10H22O	019781-26-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120424\
Data File : BF140739.D
Acq On : 04 Dec 2024 20:49
Operator : RC/JU
Sample : P5072-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-738

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.158	58.8	ng	1183540	1	6.869	402728	20.0
Propane, 1,1-di...	2.269	2.7	ng	54469	1	6.869	402728	20.0
2-Pentanone, 4-...	5.099	10.7	ng	215817	1	6.869	402728	20.0
Pentanedioic ac...	7.687	2.2	ng	57934	2	8.151	532654	20.0
Benzophenone	10.616	6.3	ng	186796	3	9.904	594219	20.0
9-Octadecenamid...	13.463	26.4	ng	517301	5	14.051	391979	20.0