

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
 Data File : BF139033.D
 Acq On : 15 Aug 2024 20:44
 Operator : RC/JU
 Sample : P3600-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VCPS-B3-081324-0-10

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: BF139033.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	17	rVB	603486	721262	75.04%	9.534%
2	3.410	219	224	232	rBV2	5349	16300	1.70%	0.215%
3	5.063	500	505	518	rVB	35917	59900	6.23%	0.792%
4	5.469	569	574	592	rBV	622525	861987	89.68%	11.394%
5	6.481	741	746	774	rBV	673406	908013	94.47%	12.003%
6	6.834	802	806	813	rBV	189963	230667	24.00%	3.049%
7	7.398	897	902	915	rBV	454129	601574	62.59%	7.952%
8	7.663	943	947	955	rBB	6933	11166	1.16%	0.148%
9	8.116	1019	1024	1037	rVB	239653	301817	31.40%	3.990%
10	8.434	1074	1078	1090	rBV	26271	41773	4.35%	0.552%
11	8.534	1090	1095	1104	rBV	13887	25087	2.61%	0.332%
12	9.186	1201	1206	1211	rBV	789493	961155	100.00%	12.705%
13	9.863	1316	1321	1327	rBV	265220	338209	35.19%	4.471%
14	9.957	1332	1337	1344	rBV	30037	44607	4.64%	0.590%
15	10.657	1451	1456	1469	rBV	416731	538711	56.05%	7.121%
16	11.357	1570	1575	1583	rBV2	250839	373281	38.84%	4.934%
17	11.880	1654	1664	1673	rBV4	15291	33740	3.51%	0.446%
18	11.969	1675	1679	1687	rVB5	6601	12560	1.31%	0.166%
19	12.422	1749	1756	1757	rBV2	11349	15703	1.63%	0.208%
20	12.439	1757	1759	1767	rVB3	12276	14886	1.55%	0.197%
21	12.569	1777	1781	1791	rBV	40892	56334	5.86%	0.745%
22	12.739	1804	1810	1815	rBV	100634	123905	12.89%	1.638%
23	12.798	1815	1820	1827	rVB	31611	46247	4.81%	0.611%
24	12.933	1838	1843	1853	rVB	493104	626819	65.22%	8.286%
25	13.069	1863	1866	1870	rVB	12136	13091	1.36%	0.173%
26	13.427	1924	1927	1932	rVB	27228	33050	3.44%	0.437%
27	13.833	1989	1996	2007	rBV9	13576	40648	4.23%	0.537%
28	13.998	2019	2024	2034	rVB2	141092	211831	22.04%	2.800%
29	14.227	2056	2063	2070	rBV2	13520	17718	1.84%	0.234%
30	14.604	2123	2127	2132	rVB	16706	20912	2.18%	0.276%
31	14.733	2145	2149	2155	rBV5	10352	17408	1.81%	0.230%
32	15.045	2196	2202	2212	rVB	13718	35349	3.68%	0.467%
33	15.345	2249	2253	2259	rBV	7298	10157	1.06%	0.134%
34	15.404	2259	2263	2267	rVV	10180	14195	1.48%	0.188%
35	15.463	2267	2273	2285	rVB	117843	185061	19.25%	2.446%

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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

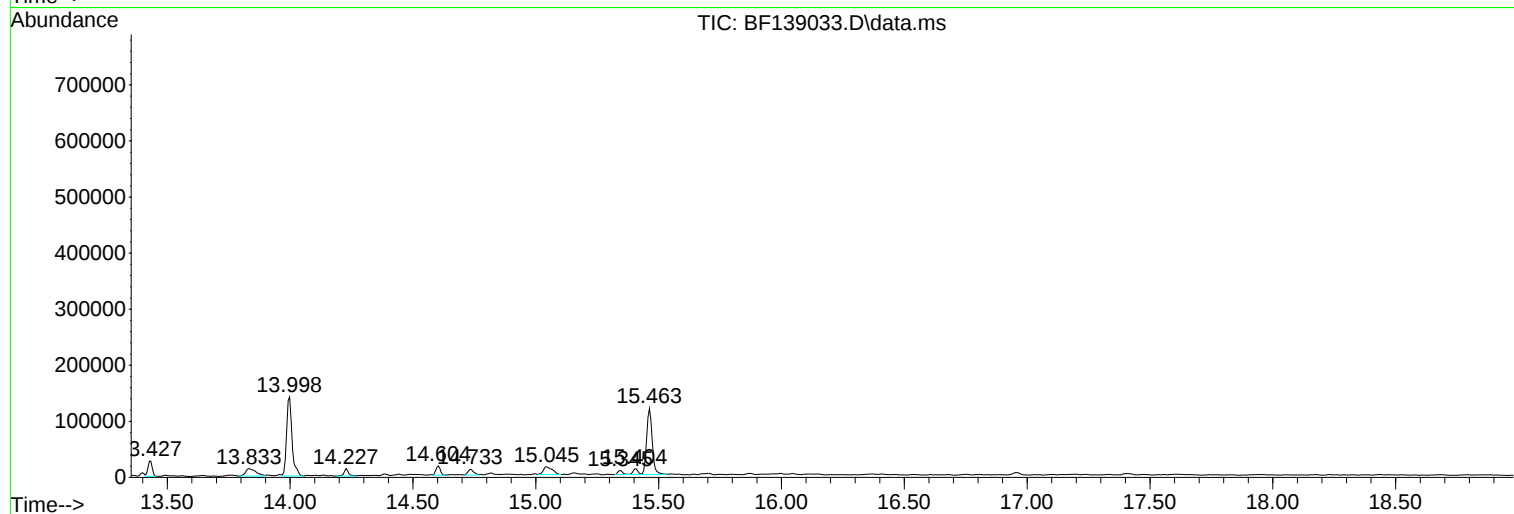
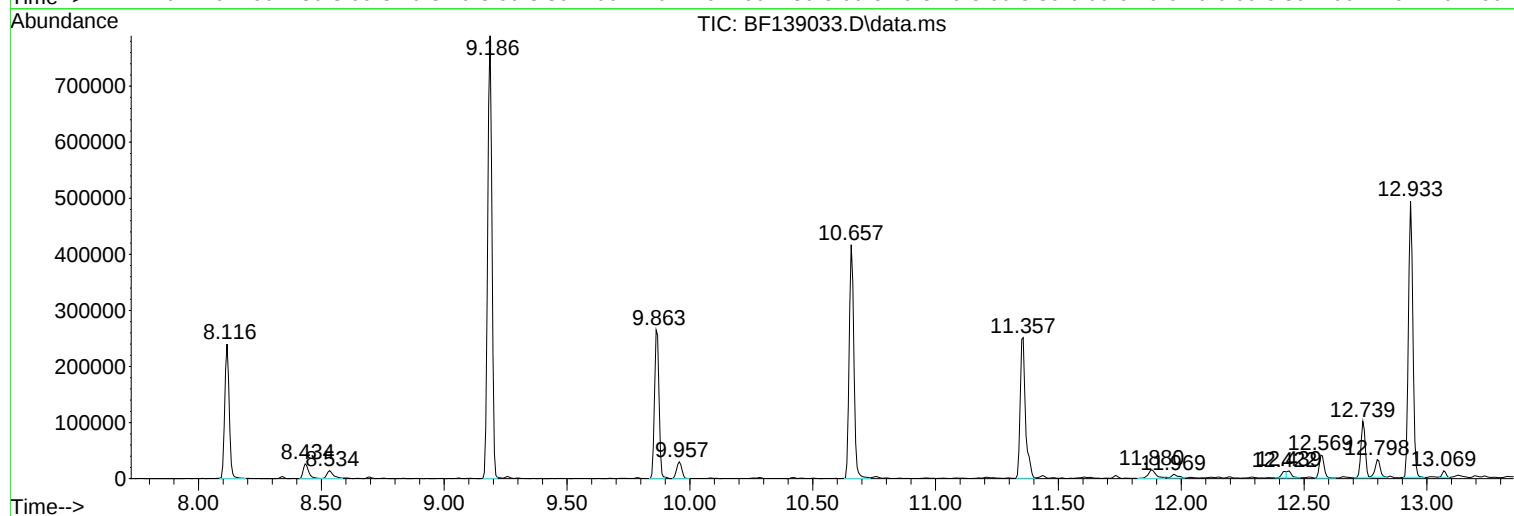
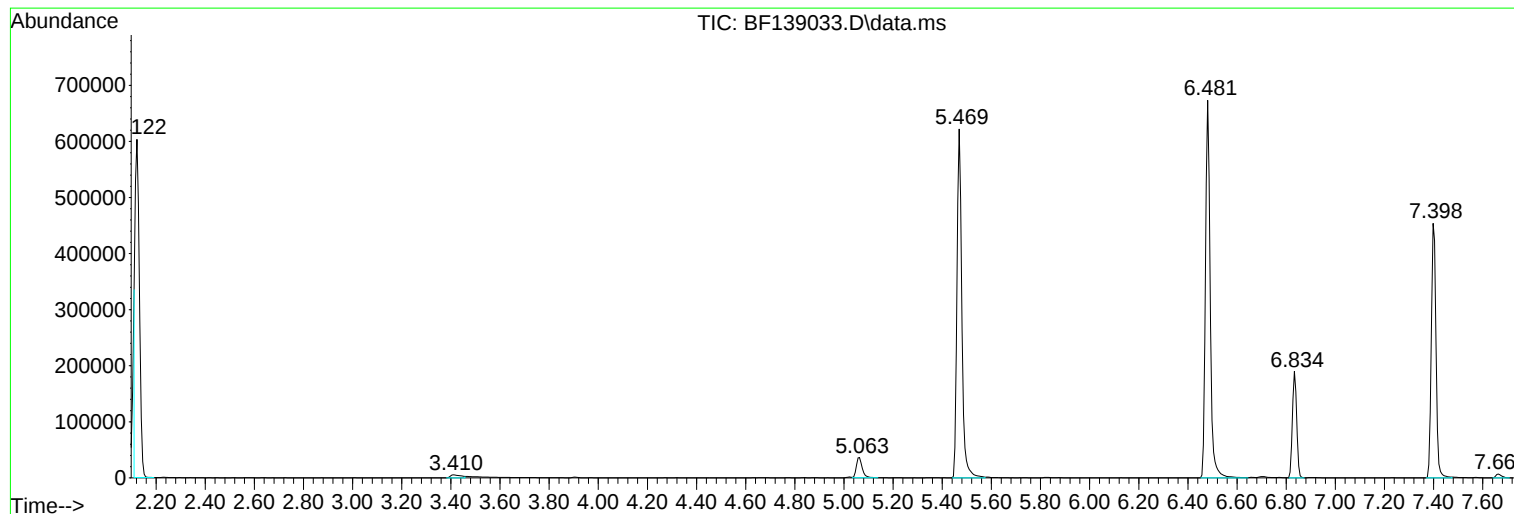
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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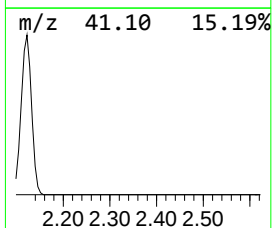
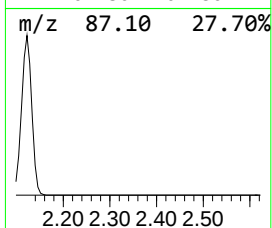
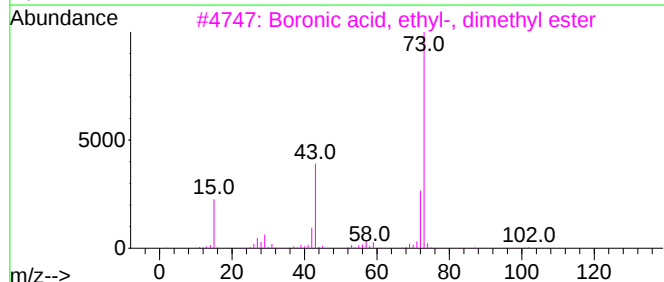
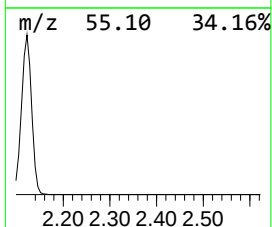
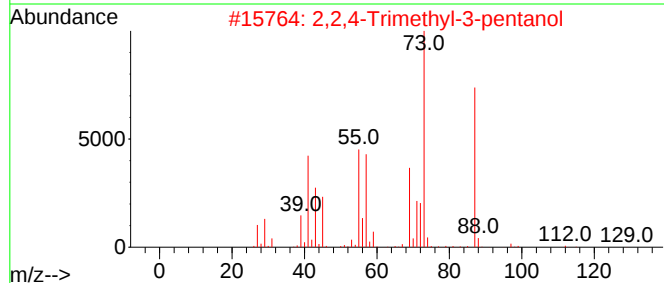
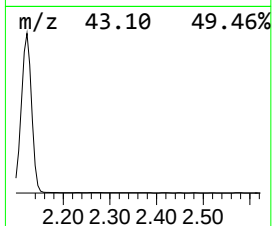
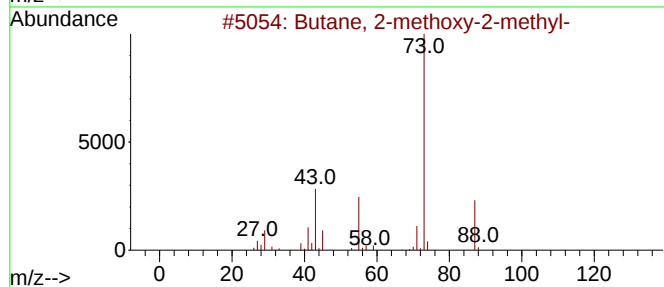
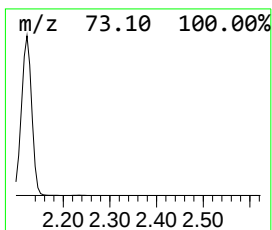
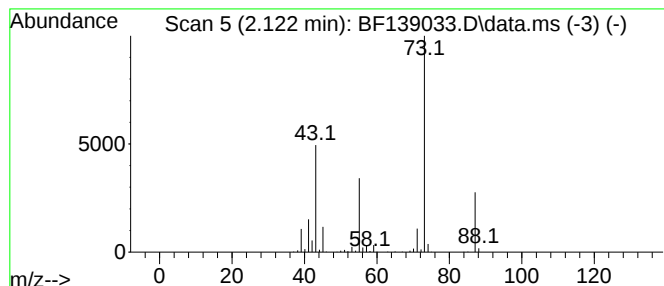
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.122	62.54 ng	721262	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	39
3			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	25
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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Instrument :
BNA_F
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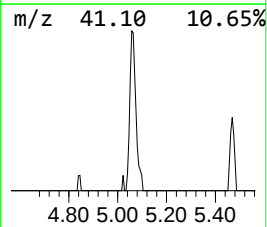
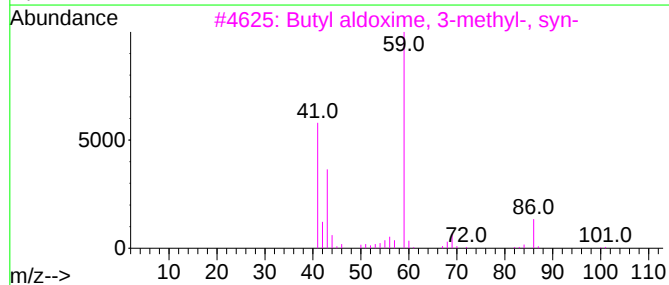
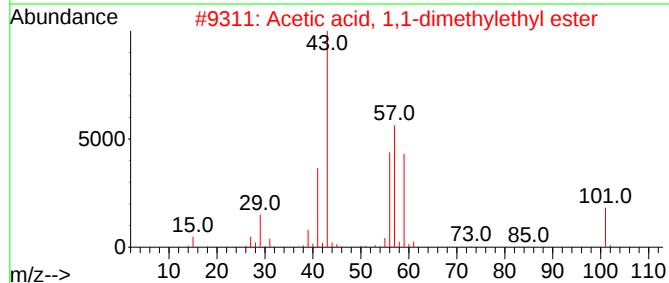
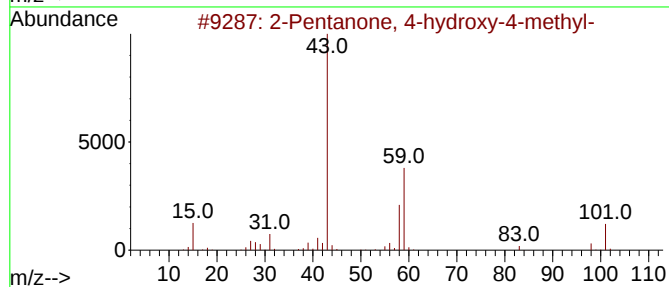
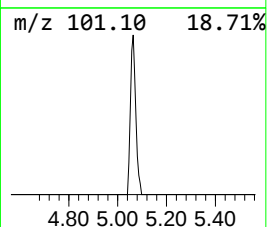
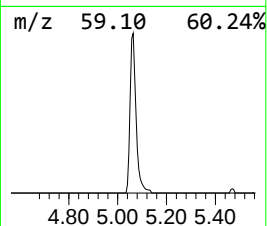
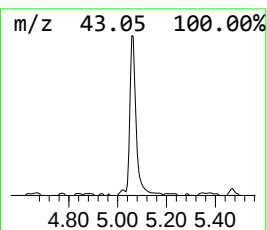
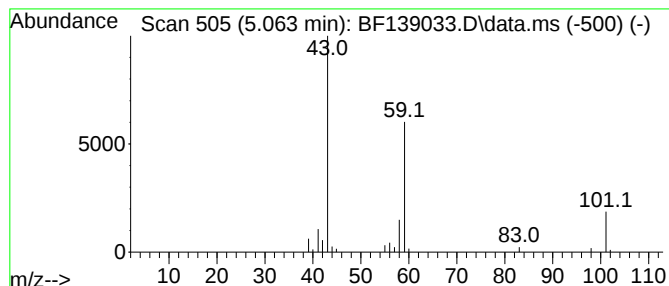
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	5.19 ng	59900	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	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
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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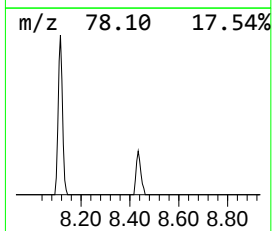
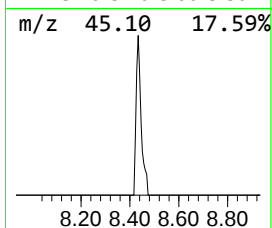
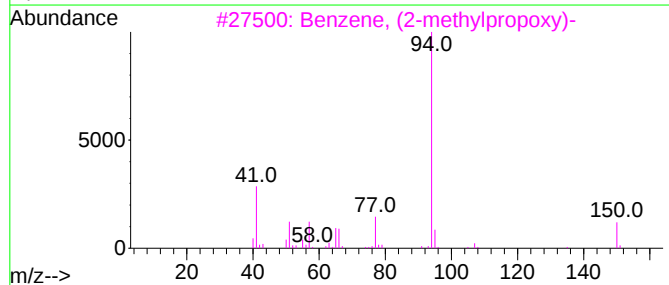
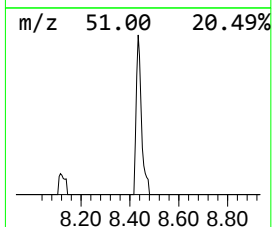
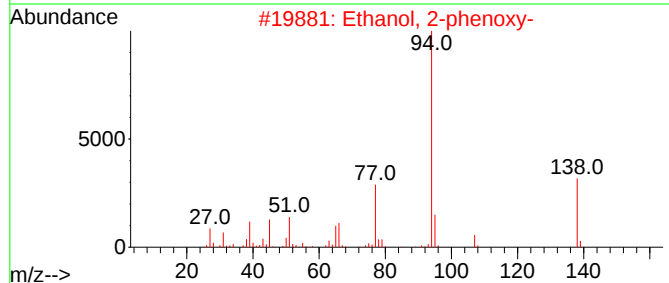
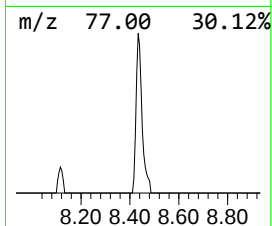
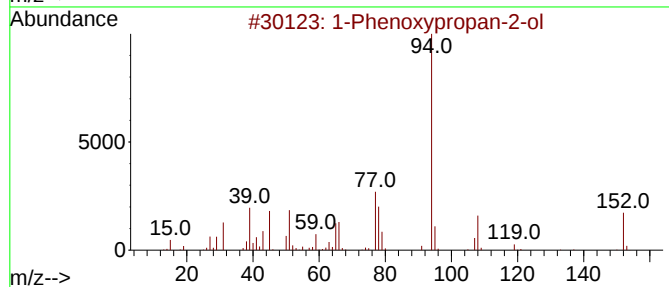
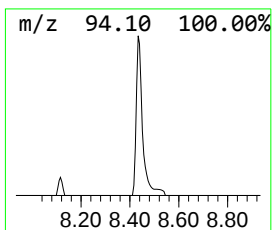
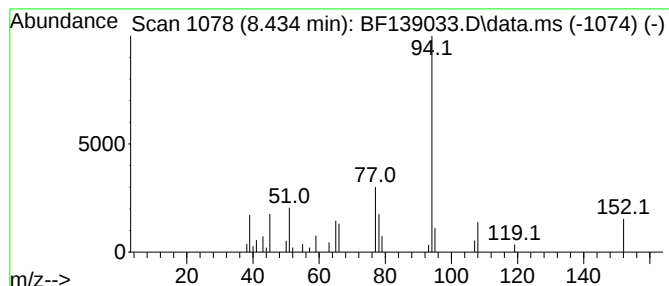
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	2.77 ng	41773	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
3			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	59
4			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	53
5			Acetic acid, phenyl ester	136	C8H8O2	000122-79-2	47



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Instrument :
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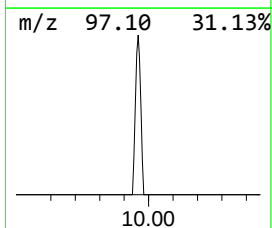
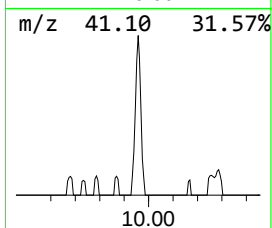
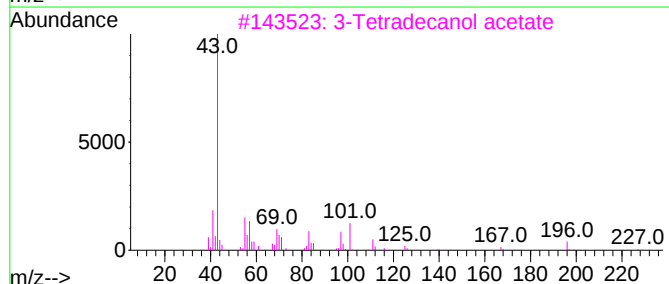
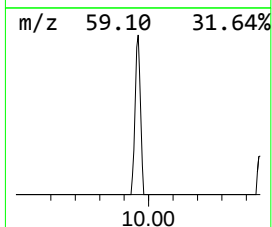
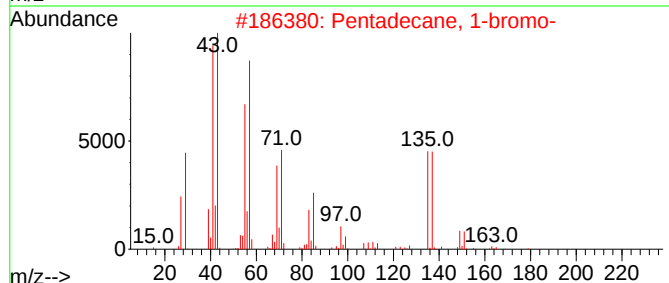
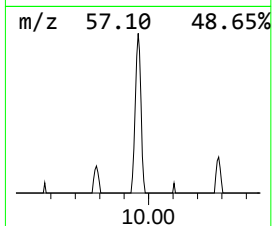
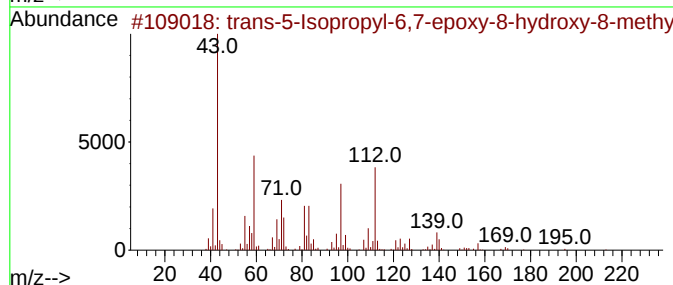
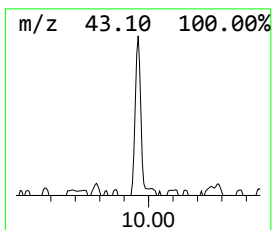
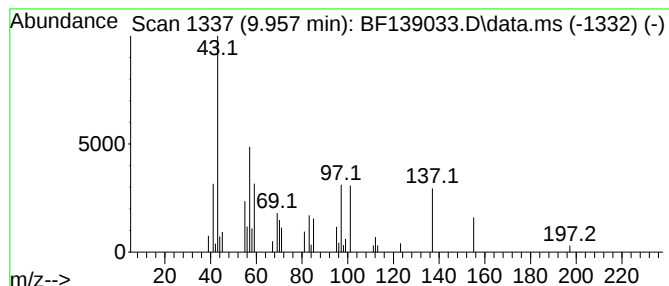
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown9.957 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.957	2.64 ng	44607	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
2			Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	10
3			3-Tetradecanol acetate	256	C16H32O2	051354-23-5	10
4			Hexanoic acid, 3-oxo-, methyl ester	144	C7H12O3	030414-54-1	10
5			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	10



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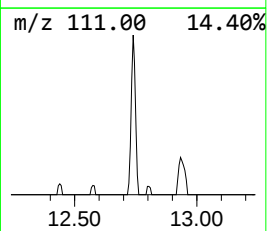
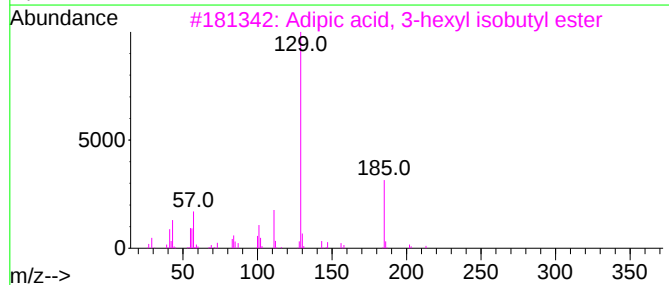
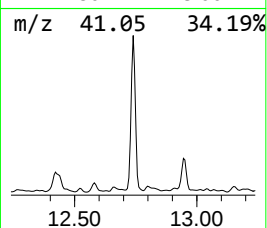
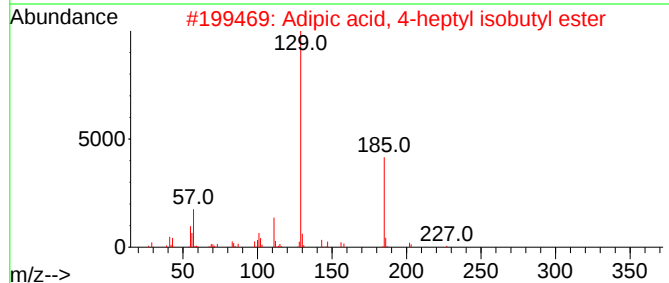
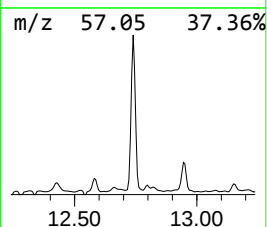
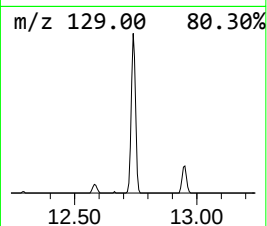
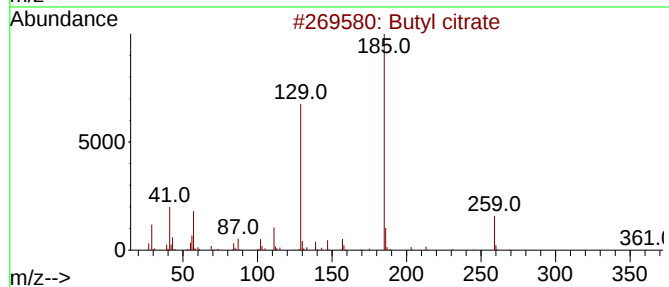
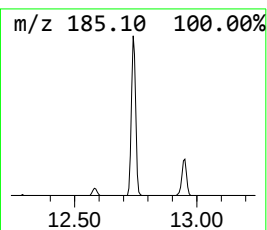
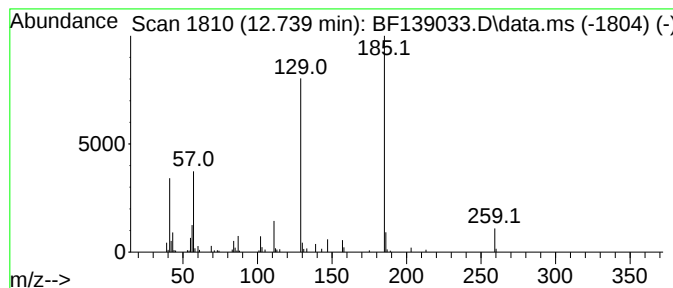
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Butyl citrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	11.70 ng	123905	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	91
2			Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	56
3			Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	56
4			Adipic acid, butyl 2-decyl ester	342	C20H38O4	1000353-59-7	50
5			Adipic acid, 2-heptyl isobutyl e...	300	C17H32O4	1000353-64-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139033.D
Acq On : 15 Aug 2024 20:44
Operator : RC/JU
Sample : P3600-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VCPS-B3-081324-0-10

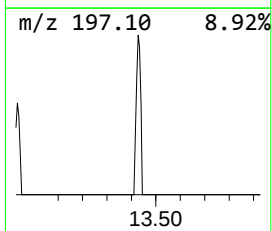
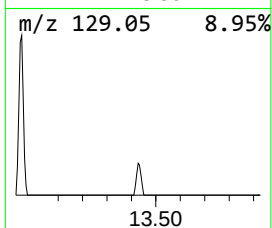
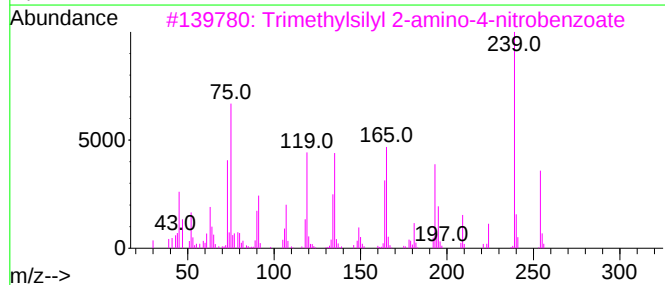
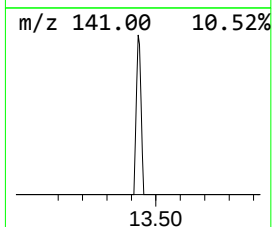
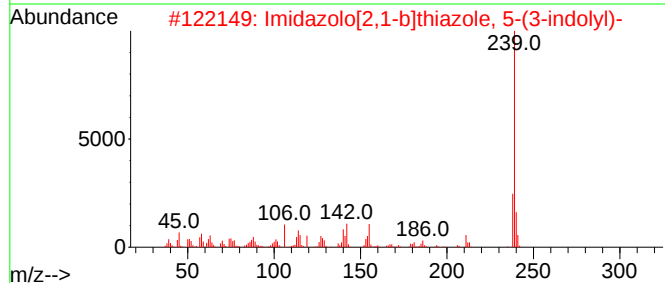
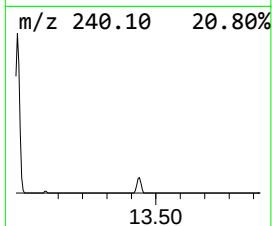
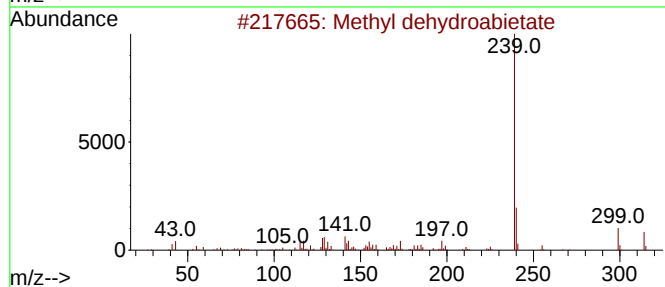
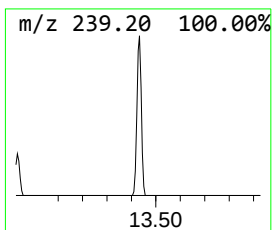
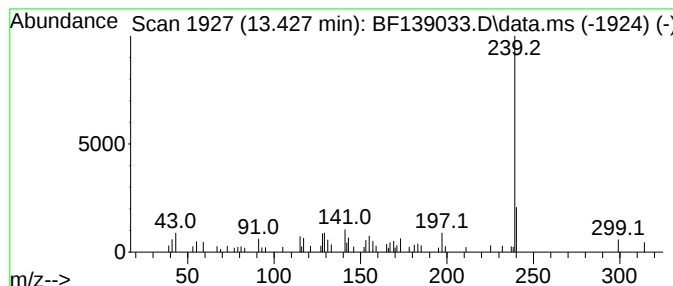
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl dehydroabietate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	3.12 ng	33050	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl dehydroabietate	314	C21H30O2	001235-74-1	95
2			Imidazolo[2,1-b]thiazole, 5-(3-i...	239	C13H9N3S	327097-37-0	64
3			Trimethylsilyl 2-amino-4-nitrobe...	254	C10H14N2O4Si	1000473-63-5	53
4			9H-Thioxanthen-9-one, 2-(1-methy...	254	C16H14O5	005495-84-1	50
5			Cobalt, (.eta.5-2,4-cyclopentadi...	239	C14H12Co	088242-61-9	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139033.D
Acq On : 15 Aug 2024 20:44
Operator : RC/JU
Sample : P3600-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VCPS-B3-081324-0-10

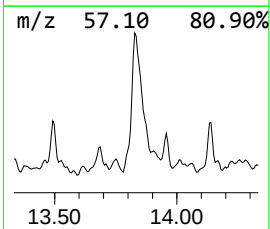
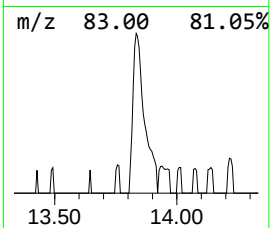
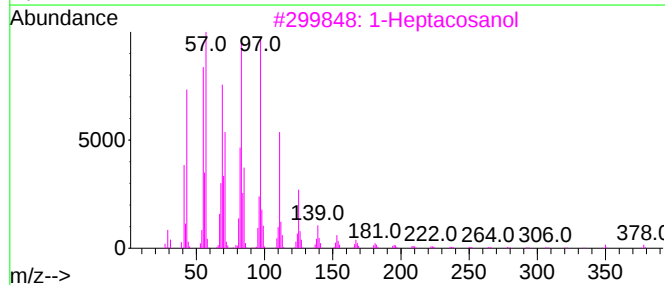
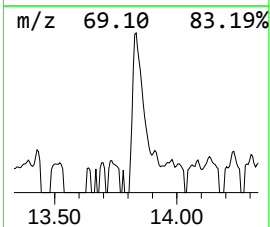
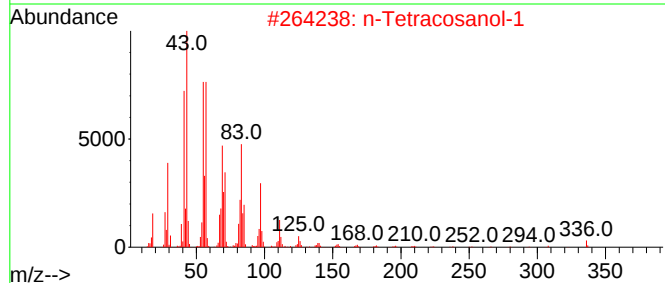
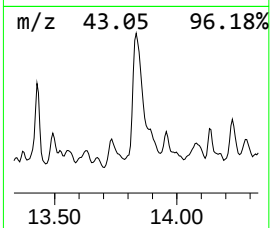
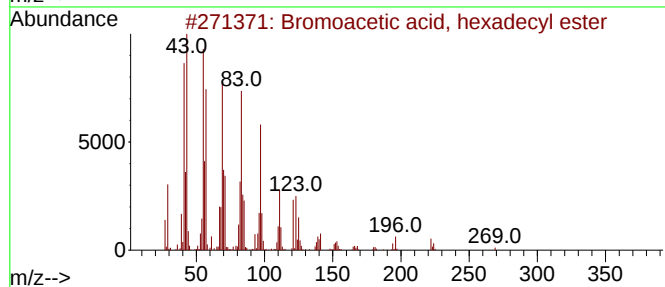
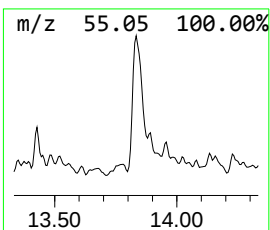
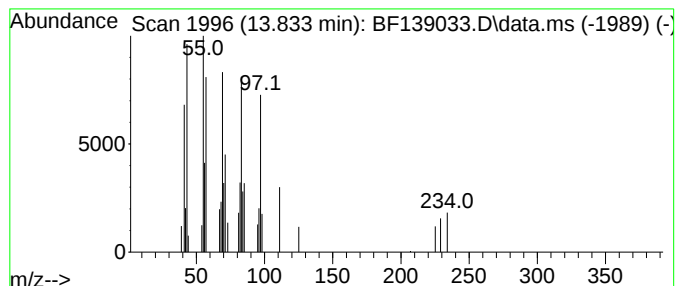
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bromoacetic acid, hexadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	3.84 ng	40648	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139033.D
Acq On : 15 Aug 2024 20:44
Operator : RC/JU
Sample : P3600-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VCPS-B3-081324-0-10

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
Butane, 2-metho...	2.122	62.5	ng	721262	1	6.834	230667	20.0
2-Pentanone, 4-...	5.063	5.2	ng	59900	1	6.834	230667	20.0
1-Phenoxypropan...	8.434	2.8	ng	41773	2	8.116	301817	20.0
unknown9.957	9.957	2.6	ng	44607	3	9.863	338209	20.0
Butyl citrate	12.739	11.7	ng	123905	5	13.998	211831	20.0
Methyl dehydroa...	13.427	3.1	ng	33050	5	13.998	211831	20.0
Bromoacetic aci...	13.833	3.8	ng	40648	5	13.998	211831	20.0