

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
 Data File : BF124314.D
 Acq On : 14 Jun 2021 19:27
 Operator : JU/CG
 Sample : M2687-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 17-B6(112-116)

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124314.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	11	16	27	rVB3	55270	76700	7.57%	1.166%
2	5.040	497	502	509	rBV	276823	329289	32.50%	5.005%
3	5.410	562	565	570	rBV	26175	30052	2.97%	0.457%
4	5.457	570	573	582	rVB	785681	675203	66.63%	10.263%
5	5.669	606	609	613	rBB	12617	11180	1.10%	0.170%
6	6.469	741	745	756	rBV	793092	701834	69.26%	10.668%
7	6.828	803	806	809	rBV	254604	193798	19.12%	2.946%
8	7.392	898	902	905	rBV	566159	457428	45.14%	6.953%
9	8.016	1005	1008	1021	rBV	56639	65292	6.44%	0.992%
10	8.110	1021	1024	1028	rBV	301724	247064	24.38%	3.755%
11	9.186	1203	1207	1211	rBV	1022450	871094	85.96%	13.240%
12	9.869	1320	1323	1327	rBV	402530	306959	30.29%	4.666%
13	10.604	1445	1448	1451	rVB	46931	35764	3.53%	0.544%
14	10.663	1454	1458	1462	rBV	602646	544392	53.72%	8.275%
15	11.357	1573	1576	1580	rBV	364094	323737	31.95%	4.921%
16	11.428	1585	1588	1591	rVB5	25342	23054	2.28%	0.350%
17	11.651	1621	1626	1633	rBV5	6799	12927	1.28%	0.196%
18	11.751	1638	1643	1645	rVB3	15581	24293	2.40%	0.369%
19	12.445	1758	1761	1765	rBV4	13415	14150	1.40%	0.215%
20	12.951	1842	1847	1850	rBV	1160778	1013336	100.00%	15.402%
21	13.427	1924	1928	1931	rVB2	26697	22106	2.18%	0.336%
22	13.486	1935	1938	1941	rVV2	19939	13878	1.37%	0.211%
23	13.980	2019	2022	2024	rBV	33059	30265	2.99%	0.460%
24	14.010	2024	2027	2030	rVB	301325	264014	26.05%	4.013%
25	14.268	2067	2071	2073	rBV4	8498	11660	1.15%	0.177%
26	14.633	2130	2133	2136	rBV2	32282	30363	3.00%	0.462%
27	14.763	2152	2155	2161	rBV5	25166	24848	2.45%	0.378%
28	15.486	2274	2278	2288	rVB	177362	224452	22.15%	3.412%

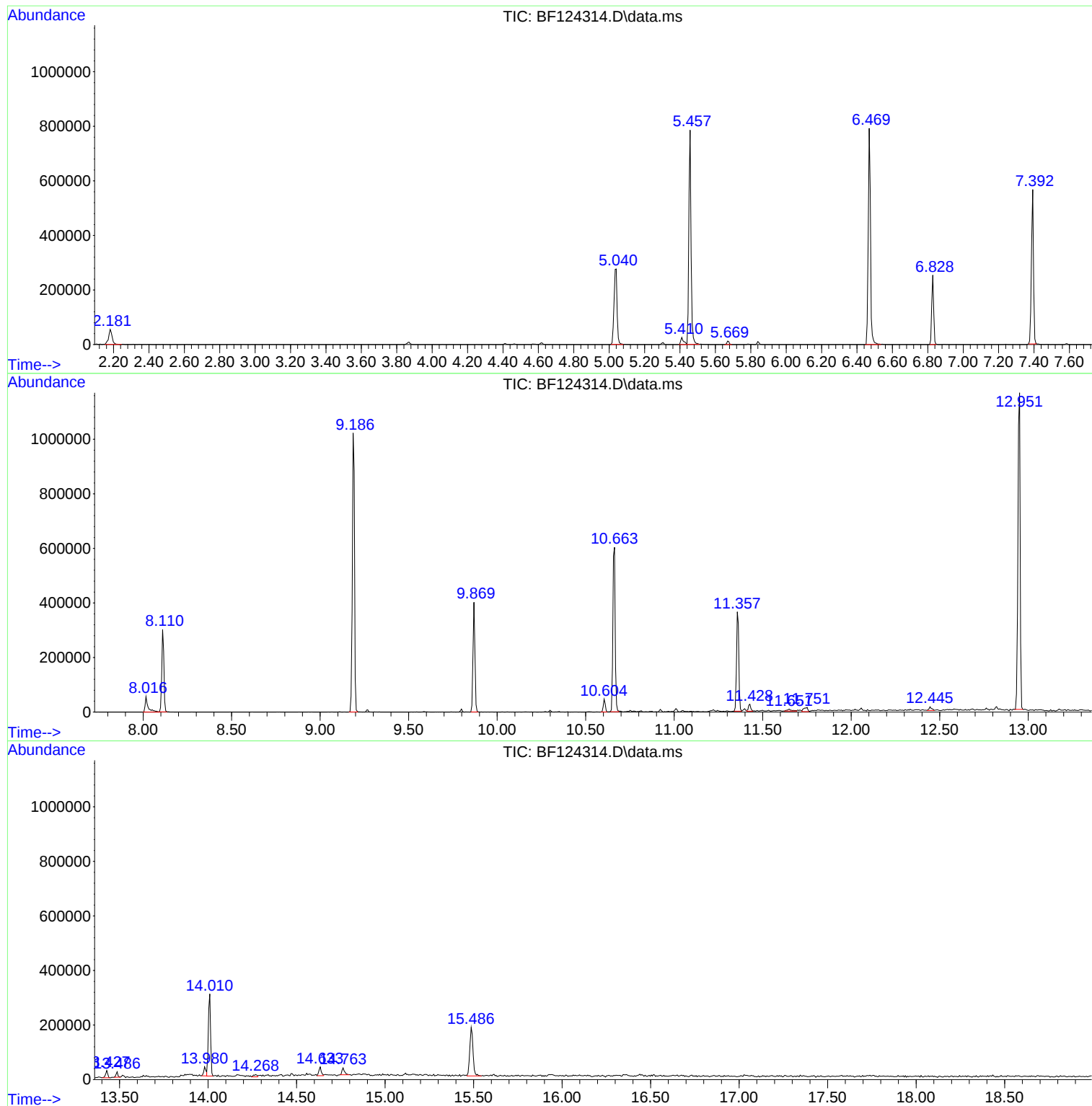
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Instrument :
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ClientSampleId :
17-B6(112-116)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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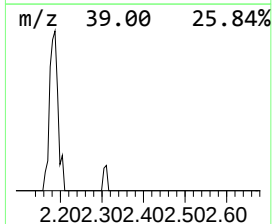
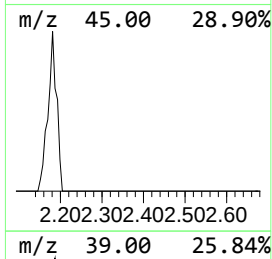
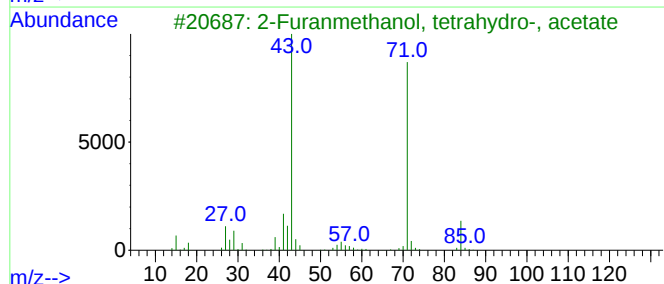
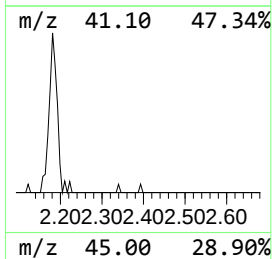
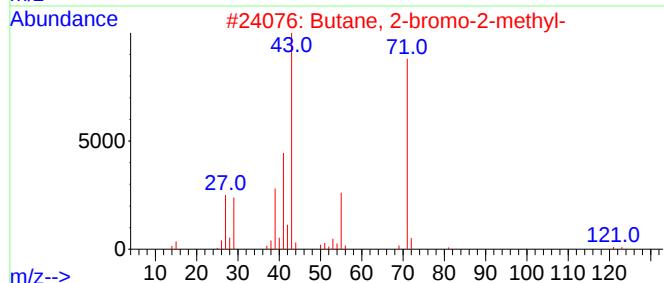
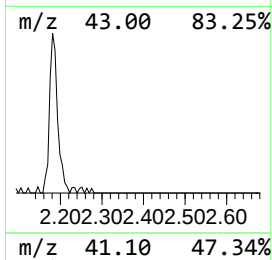
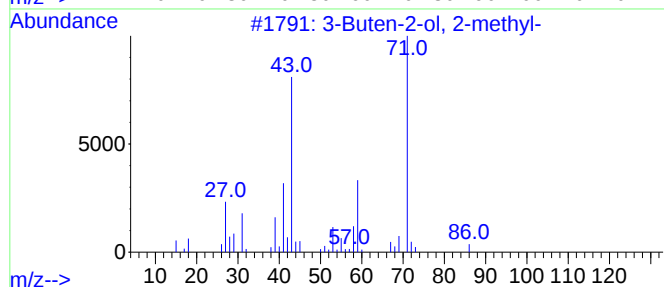
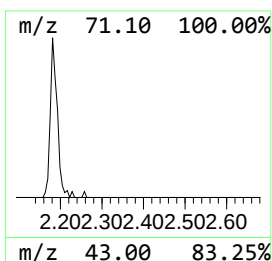
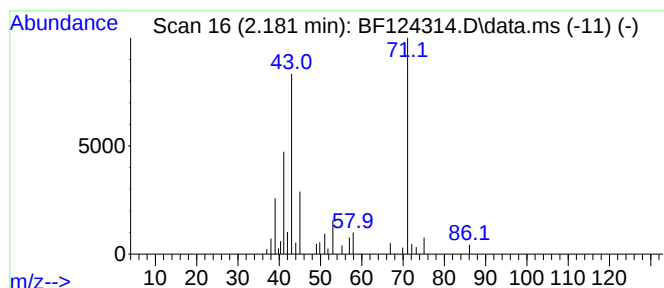
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Buten-2-ol, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	7.92 ng	76700	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	53
2			Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	50
3			2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	50
4			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	50
5			Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	50



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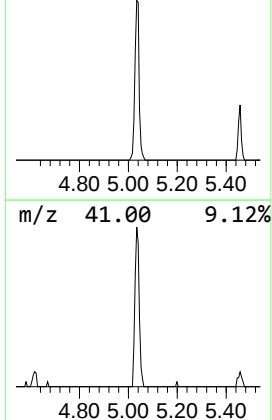
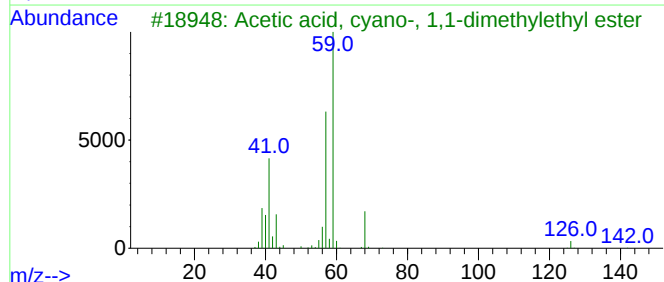
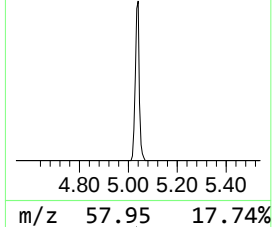
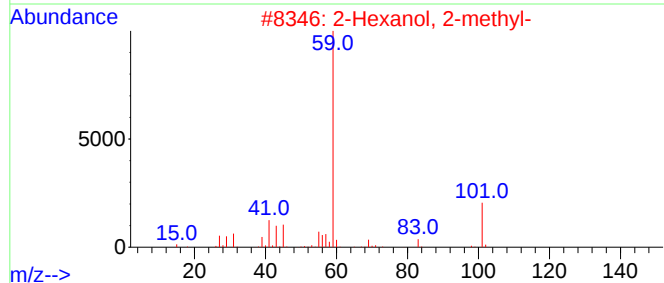
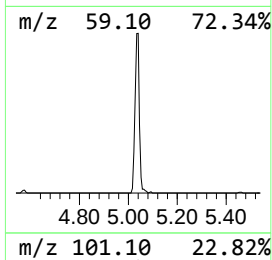
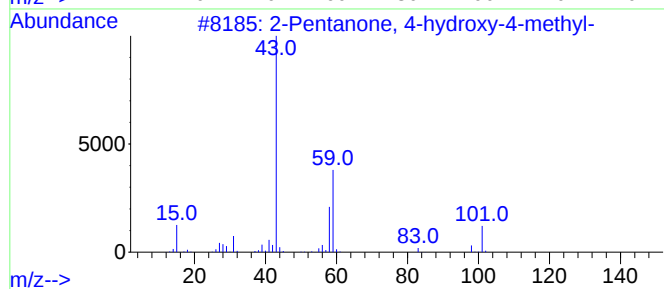
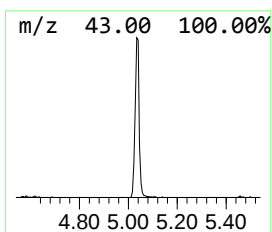
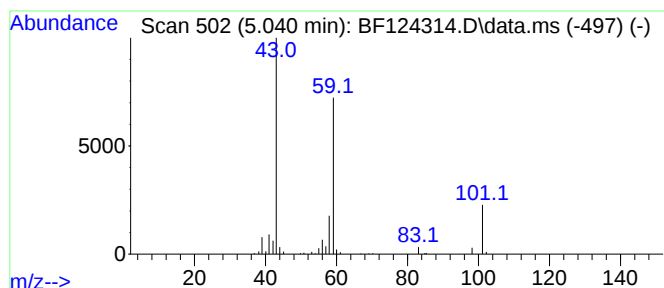
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	33.98 ng	329289	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5			Propanoic acid, 3-nitro-, methyl...	133	C4H7NO4	020497-95-4	17



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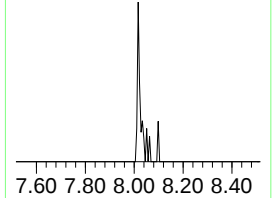
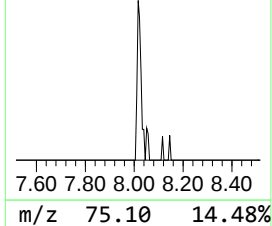
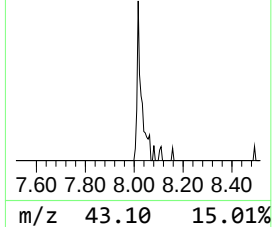
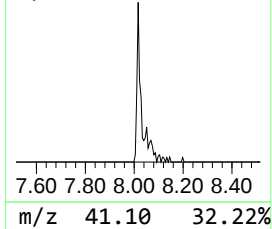
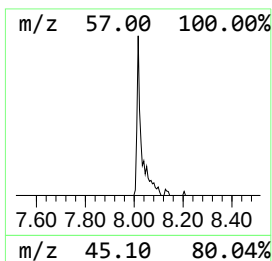
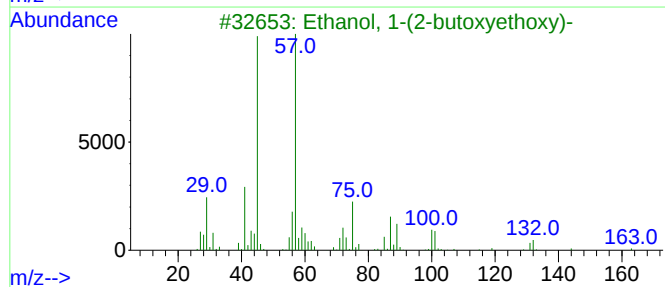
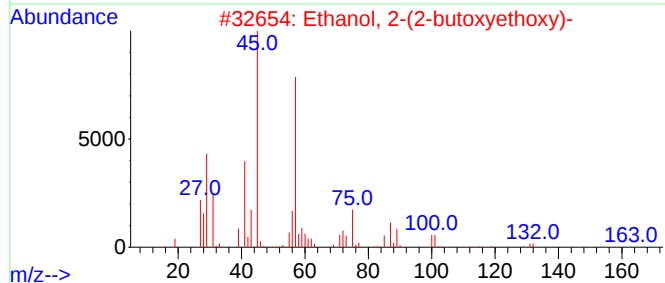
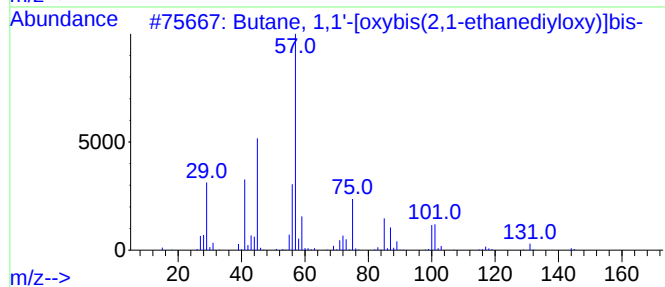
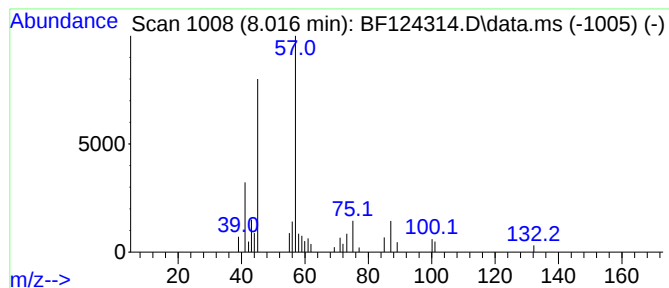
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 1,1'-[oxybis(2,1-et... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	5.29 ng	65292	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	78
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	56
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	40



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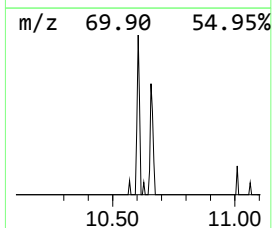
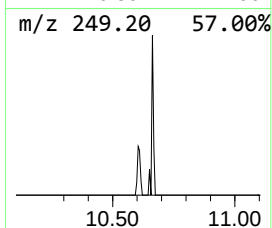
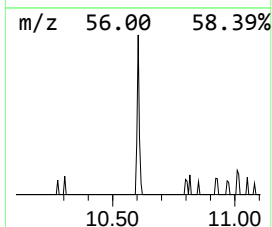
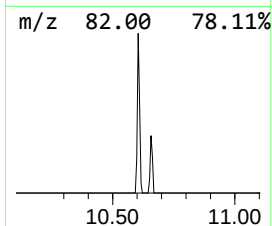
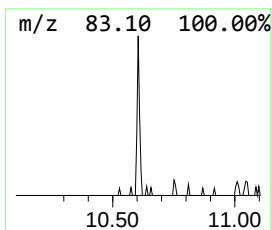
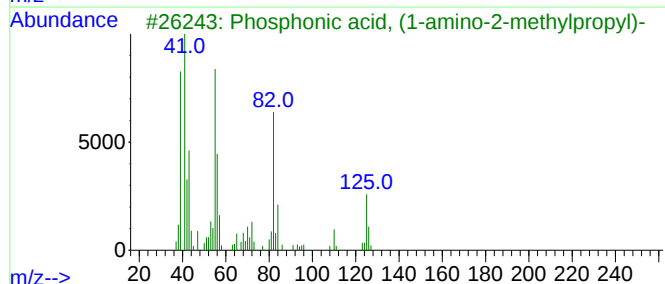
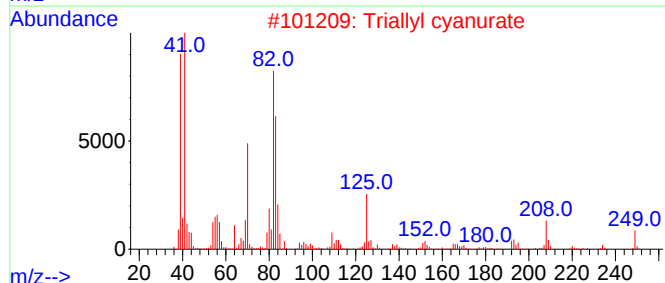
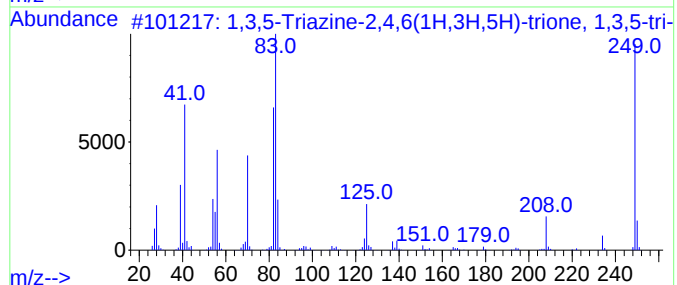
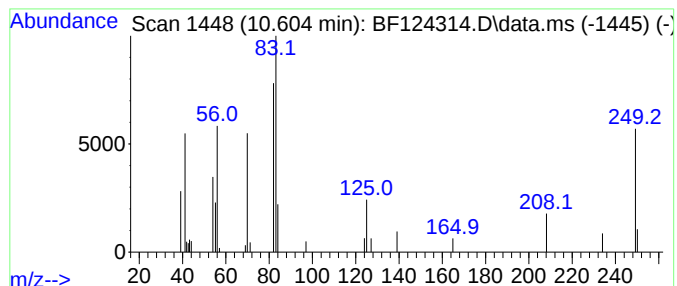
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Peak Number 4 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	2.33 ng	35764	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	94
2			Triallyl cyanurate	249	C12H15N3O3	000101-37-1	38
3			Phosphonic acid, (1-amino-2-meth...	153	C4H12NO3P	018108-24-2	12
4			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	9
5			Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	9



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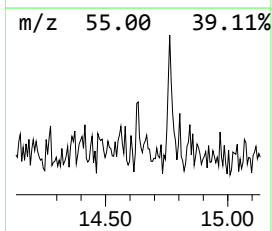
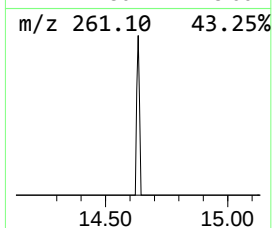
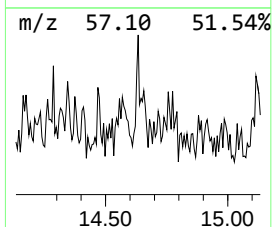
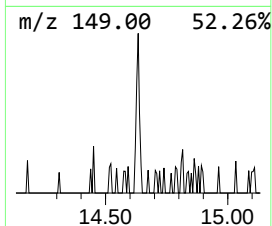
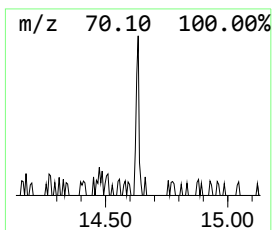
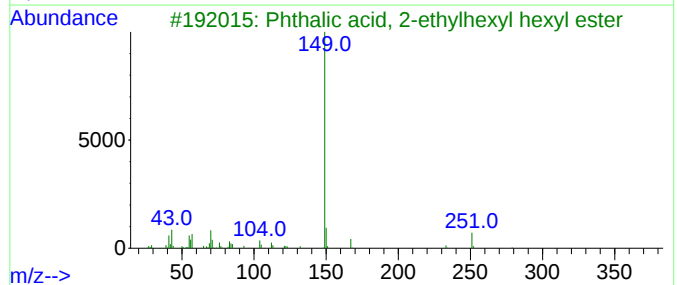
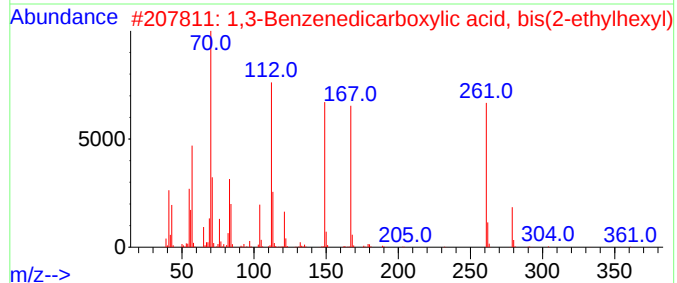
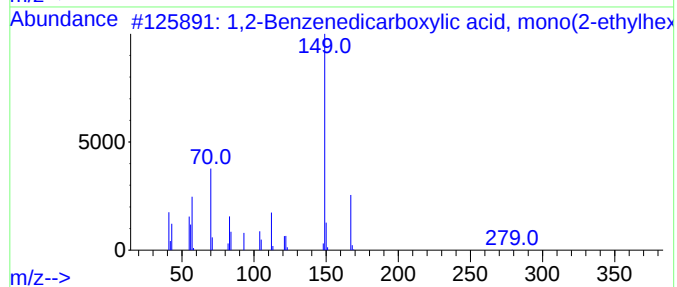
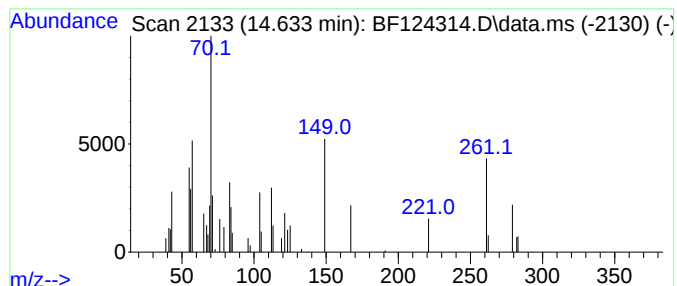
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Peak Number 5 unknown14.633 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	2.30 ng	30363	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	47
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
3			Phthalic acid, 2-ethylhexyl hexy...	362	C22H34O4	1000309-02-5	35
4			Carbonic acid, propargyl 2-ethyl...	212	C12H20O3	1000357-90-9	35
5			3-Chloropropionic acid, 2-ethylh...	220	C11H21ClO2	091369-31-2	35



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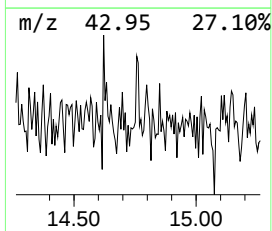
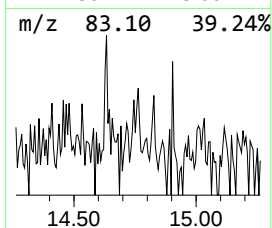
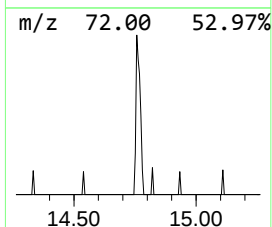
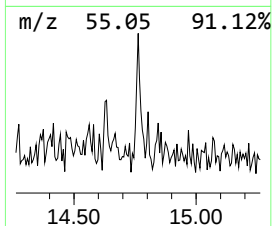
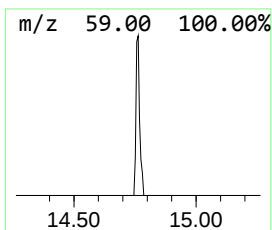
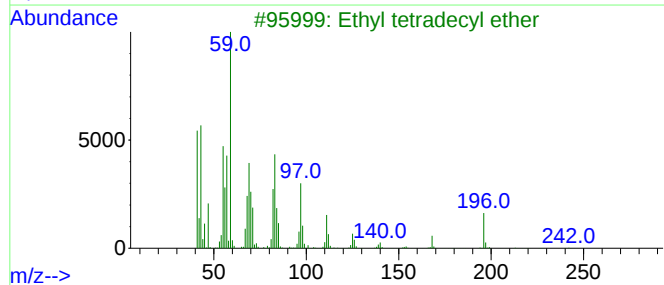
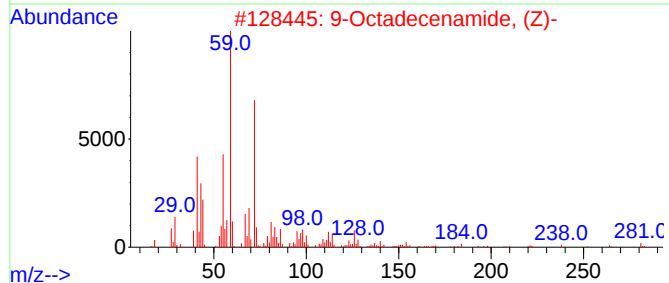
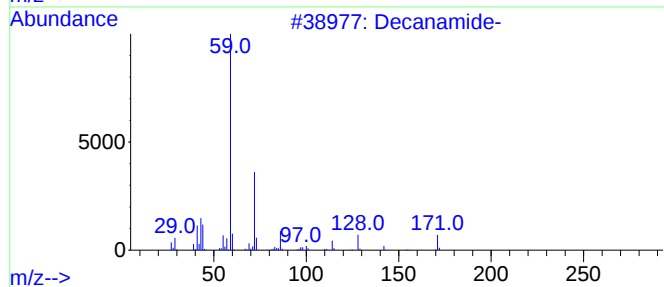
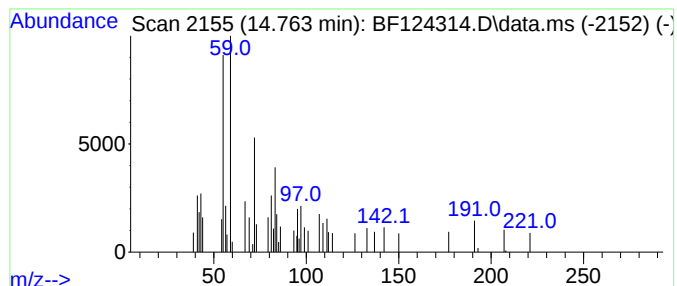
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.763 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	2.21 ng	24848	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanamide-	171	C10H21NO	002319-29-1	38
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	38
3			Ethyl tetradecyl ether	242	C16H34O	1000130-99-7	37
4			3-Pentenoic acid, methyl ester	114	C6H10O2	000818-58-6	35
5			Dodecanamide	199	C12H25NO	001120-16-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124314.D
Acq On : 14 Jun 2021 19:27
Operator : JU/CG
Sample : M2687-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(112-116)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Buten-2-ol, 2...	2.181	7.9	ng	76700	1	6.828	193798	20.0
2-Pentanone, 4-...	5.040	34.0	ng	329289	1	6.828	193798	20.0
Butane, 1,1'-[o...	8.016	5.3	ng	65292	2	8.110	247064	20.0
1,3,5-Triazine-...	10.604	2.3	ng	35764	3	9.869	306959	20.0
unknown14.633	14.633	2.3	ng	30363	5	14.010	264014	20.0
unknown14.763	14.763	2.2	ng	24848	6	15.486	224452	20.0