

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
 Data File : BF124053.D
 Acq On : 25 May 2021 19:29
 Operator : JU/CG
 Sample : M2502-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SA-01-052421

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-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124053.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	18	27	34	rBV	741665	926205	46.28%	6.520%
2	2.352	41	45	51	rVB	48487	55072	2.75%	0.388%
3	5.128	511	517	525	rVB	488556	617329	30.85%	4.346%
4	5.522	579	584	587	rBV	1632739	1638966	81.90%	11.538%
5	5.910	647	650	655	rVB	55167	44707	2.23%	0.315%
6	6.522	748	754	757	rBV	1600338	1655611	82.73%	11.655%
7	6.893	813	817	821	rBV	574480	452983	22.64%	3.189%
8	7.457	907	913	916	rBV	1216135	1122408	56.09%	7.902%
9	8.175	1029	1035	1039	rBV	635002	552435	27.61%	3.889%
10	9.251	1213	1218	1222	rBV	2121489	2001188	100.00%	14.088%
11	9.645	1281	1285	1288	rBV	126466	118951	5.94%	0.837%
12	9.934	1327	1334	1338	rBV	752368	597124	29.84%	4.204%
13	10.722	1464	1468	1471	rBV	1309272	1091464	54.54%	7.684%
14	10.845	1485	1489	1493	rVB3	19776	26943	1.35%	0.190%
15	11.422	1583	1587	1590	rBV	611385	504378	25.20%	3.551%
16	11.445	1590	1591	1593	rVB	38976	20633	1.03%	0.145%
17	11.945	1673	1676	1679	rBV4	44296	43047	2.15%	0.303%
18	12.122	1703	1706	1711	rBV6	10293	20311	1.01%	0.143%
19	12.516	1771	1773	1778	rVB5	20850	22511	1.12%	0.158%
20	12.639	1791	1794	1799	rVB	36024	36563	1.83%	0.257%
21	12.863	1830	1832	1834	rBV	33550	31859	1.59%	0.224%
22	13.010	1852	1857	1860	rBV	1630194	1357789	67.85%	9.559%
23	13.757	1982	1984	1988	rBV5	25795	37050	1.85%	0.261%
24	13.898	2005	2008	2009	rBV	36280	34547	1.73%	0.243%
25	13.927	2009	2013	2021	rVB2	231199	346430	17.31%	2.439%
26	14.069	2031	2037	2040	rBV	370549	386208	19.30%	2.719%
27	14.580	2120	2124	2129	rBV6	44688	83166	4.16%	0.585%
28	15.192	2226	2228	2232	rVB5	35937	38640	1.93%	0.272%
29	15.563	2286	2291	2295	rBV	266473	340352	17.01%	2.396%

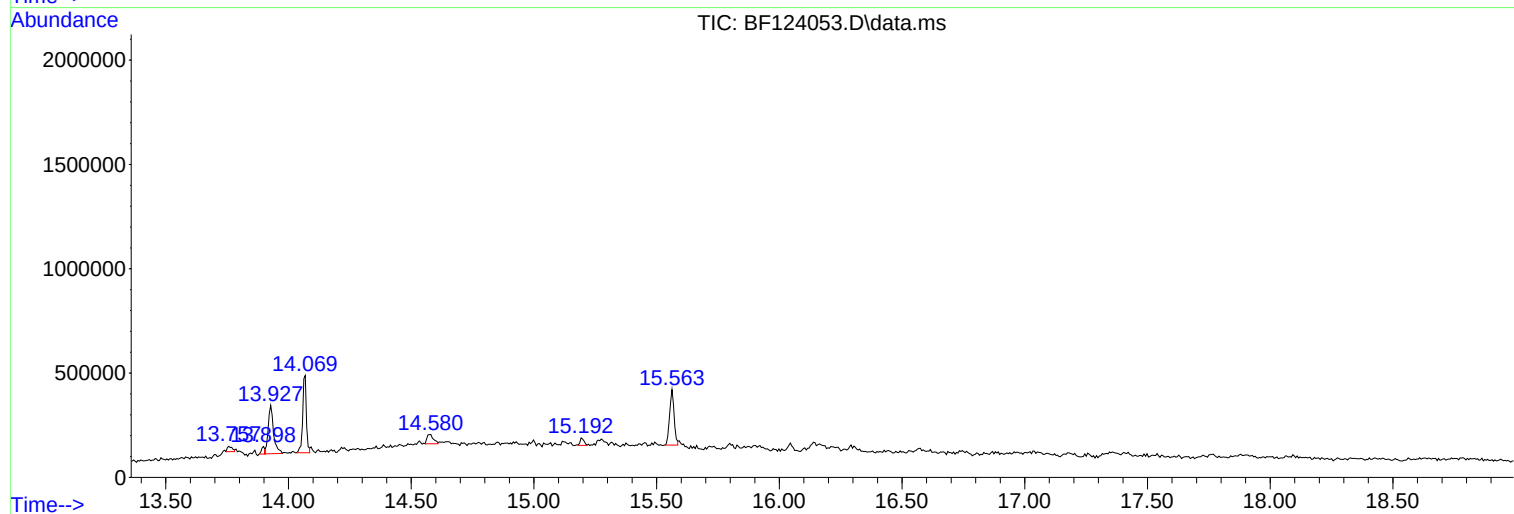
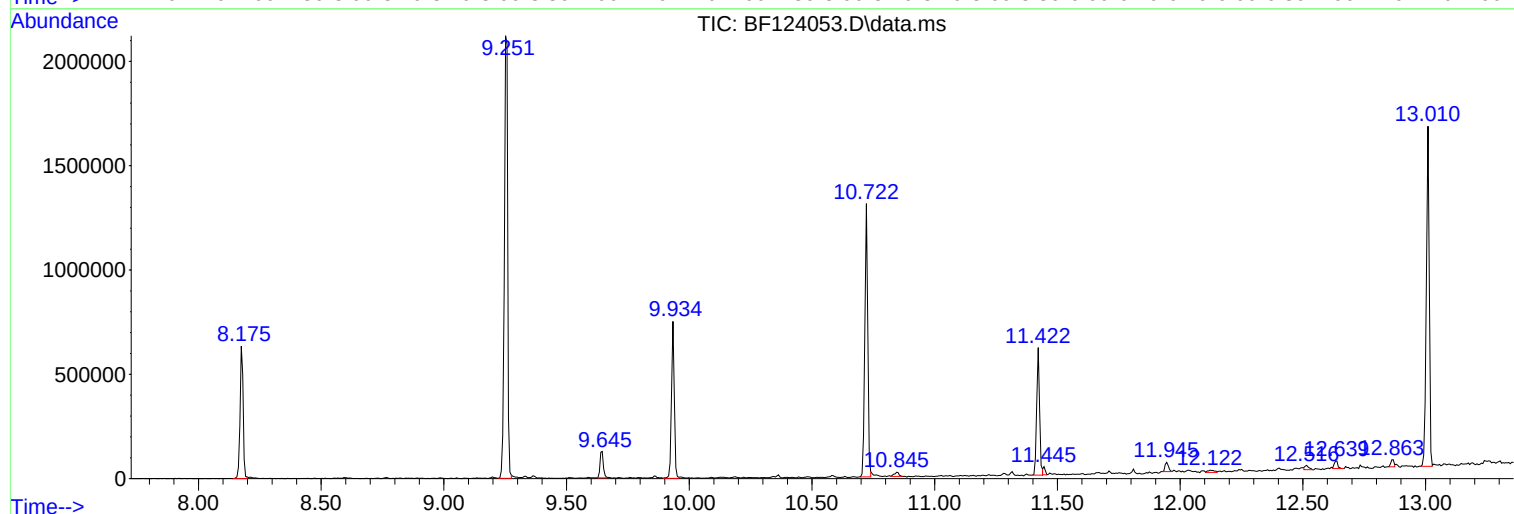
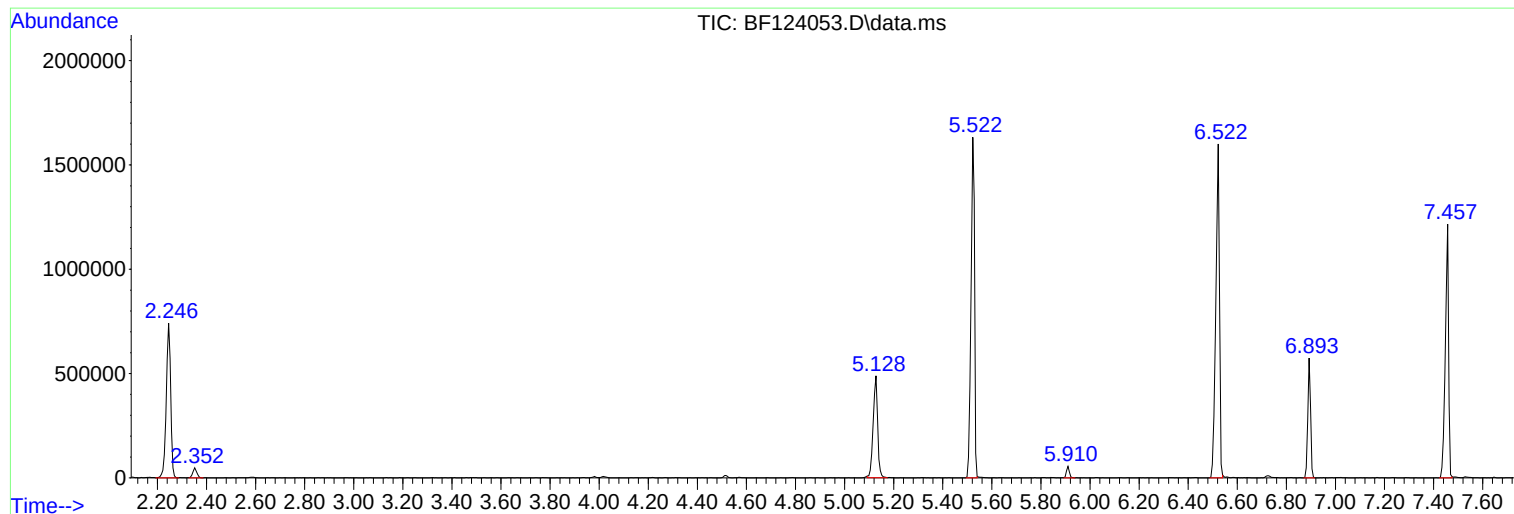
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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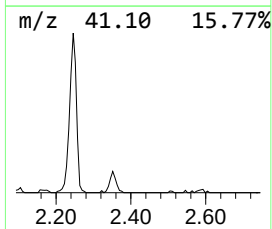
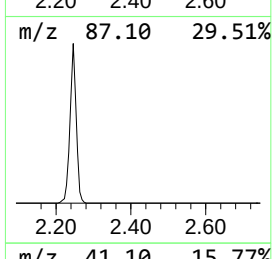
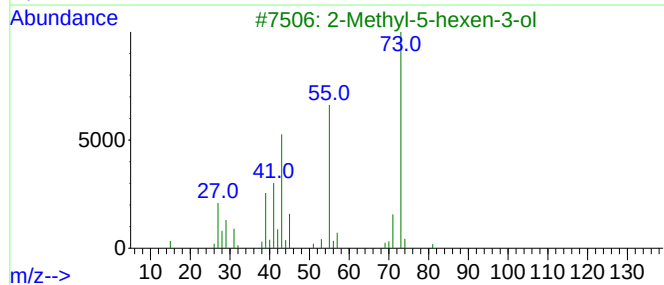
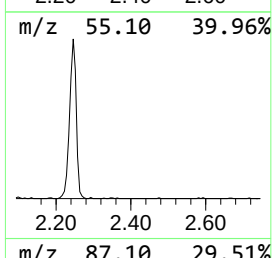
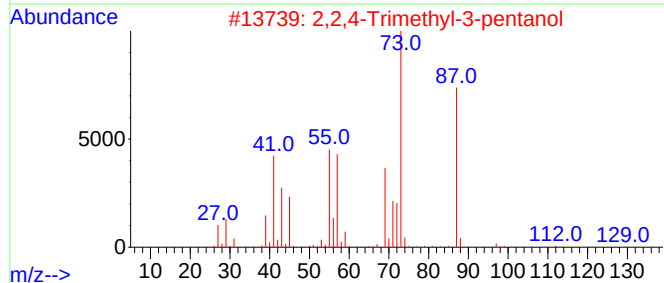
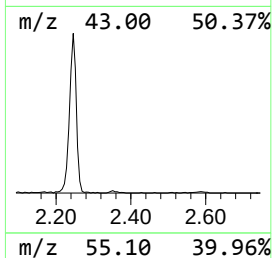
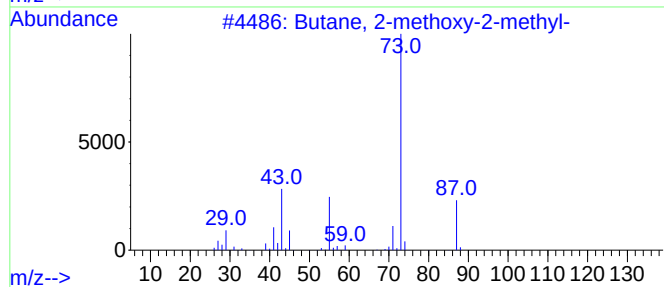
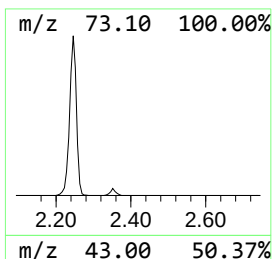
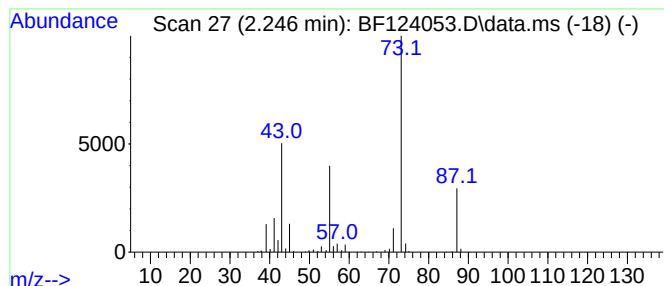
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.246	40.89 ng	926205	1,4-Dichlorobenzene-d4	6.893

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			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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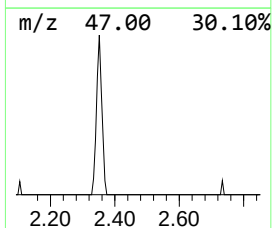
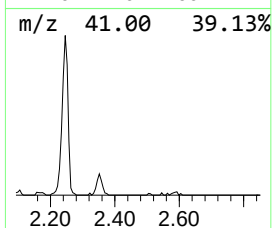
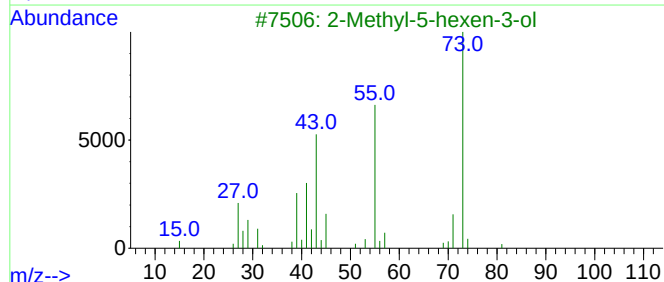
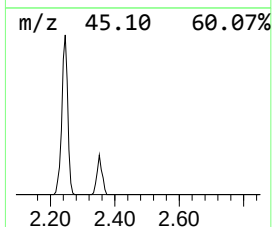
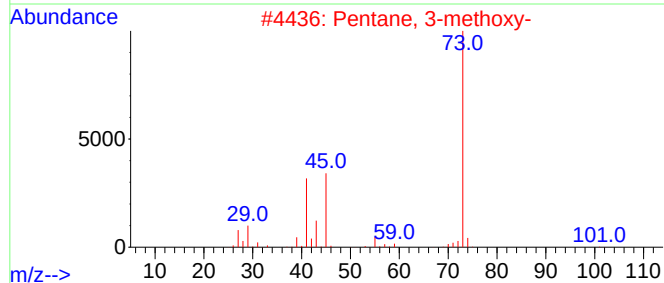
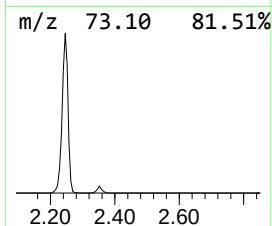
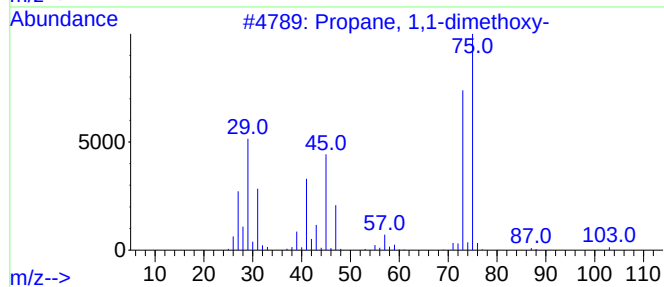
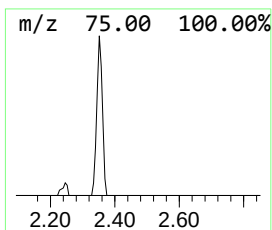
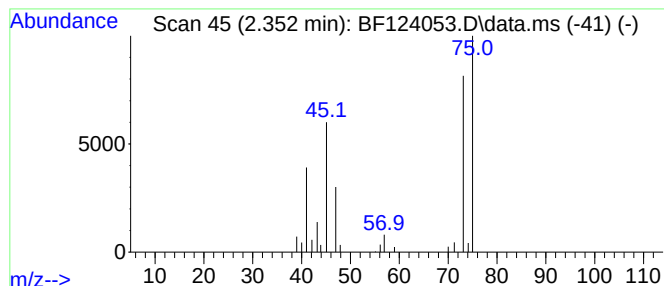
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.352	2.43 ng	55072	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Hydrazine, propyl-	74	C3H10N2	005039-61-2	9



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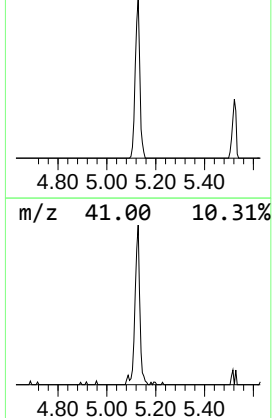
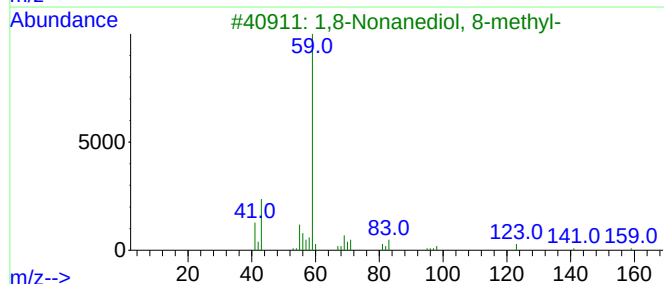
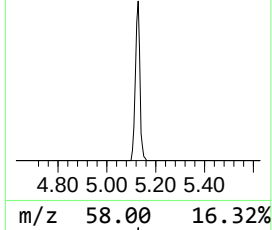
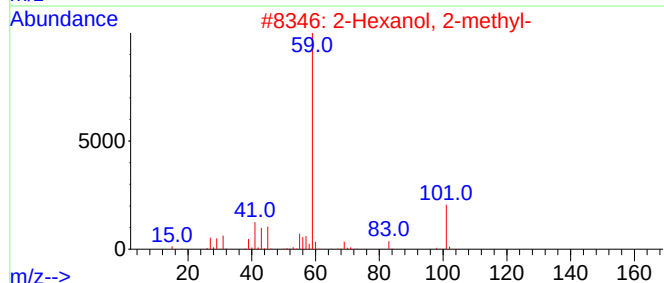
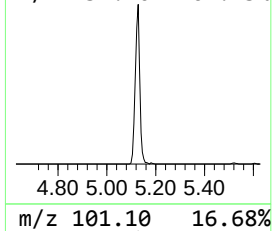
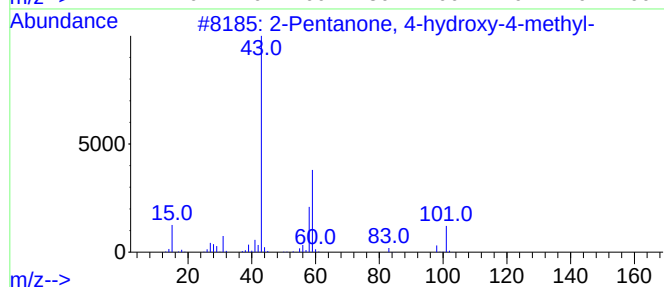
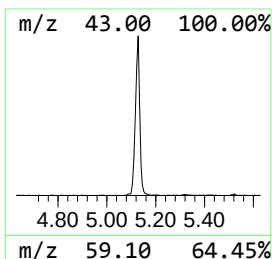
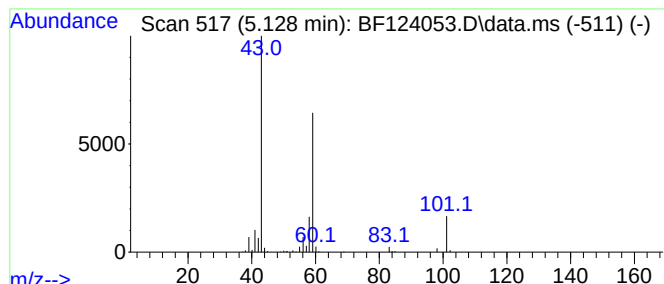
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	27.26 ng	617329	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4			Acetone	58	C3H6O	000067-64-1	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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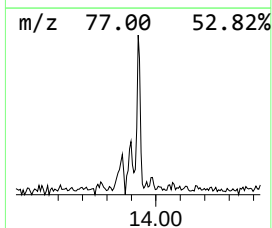
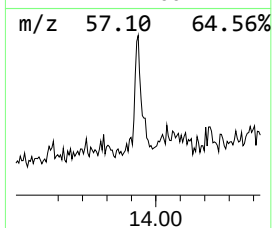
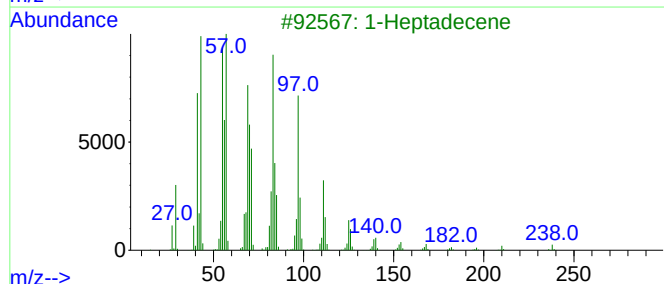
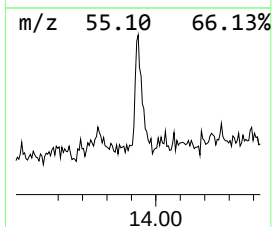
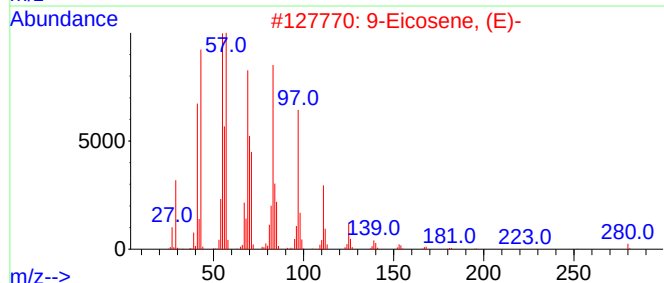
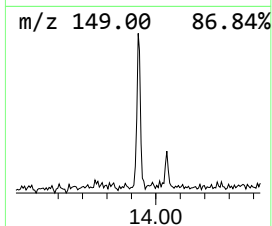
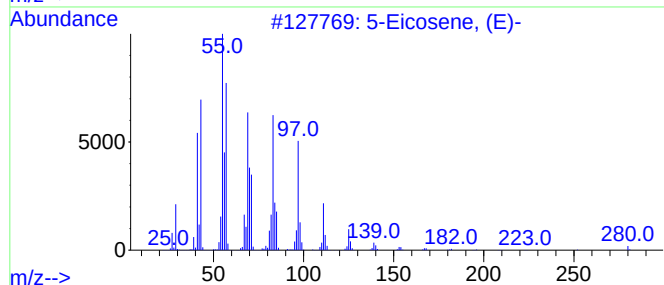
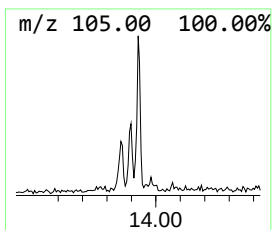
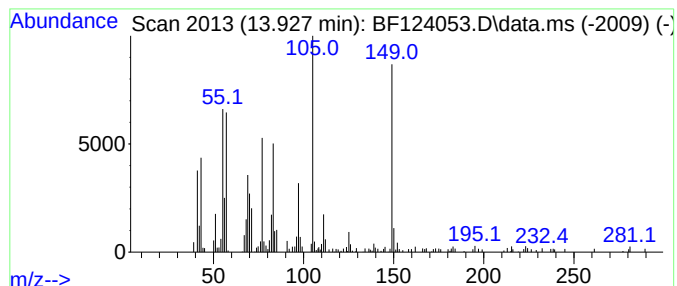
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	17.94 ng	346430	Chrysene-d12	14.069

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	60
2		9-Eicosene, (E)-	280	C20H40	074685-29-3	47
3		1-Heptadecene	238	C17H34	006765-39-5	42
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	35
5		1-Docosene	308	C22H44	001599-67-3	35



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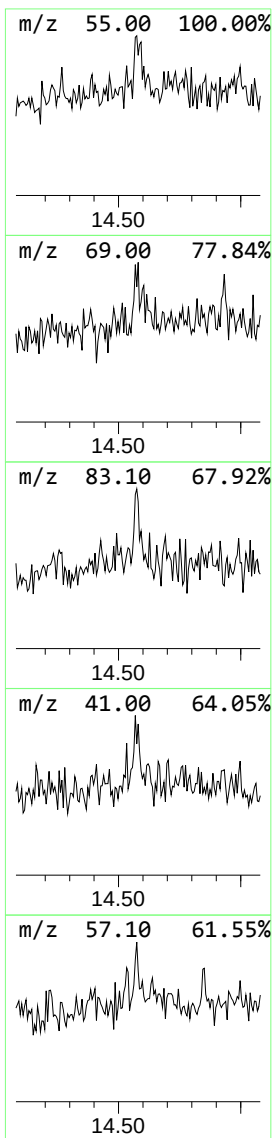
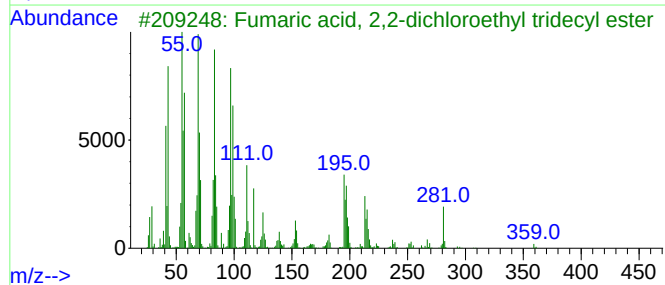
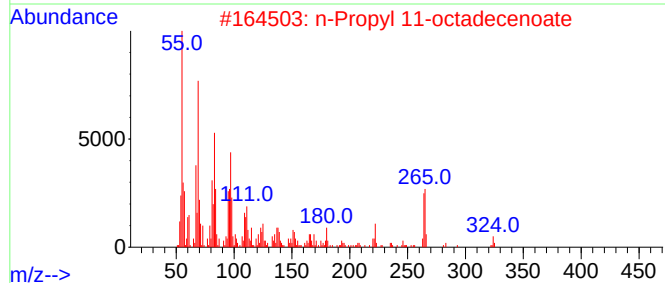
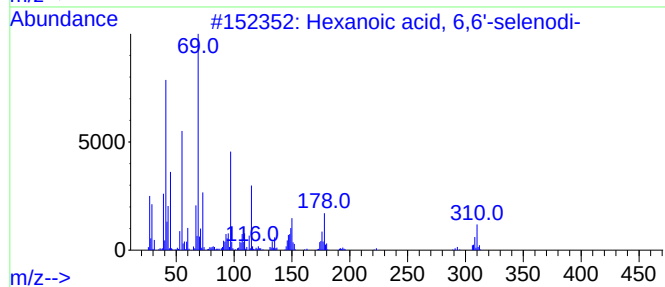
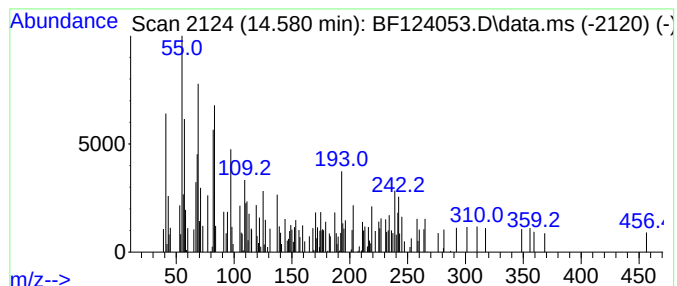
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Peak Number 5 Hexanoic acid, 6,6'-selenodi- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	4.31 ng	83166	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 6,6'-selenodi-	310	C12H22O4Se	022676-16-0	50
2			n-Propyl 11-octadecenoate	324	C21H40O2	1000336-71-7	47
3			Fumaric acid, 2,2-dichloroethyl ...	394	C19H32Cl2O4	1000348-58-1	38
4			1-Bromo-11-iodoundecane	360	C11H22BrI	139123-69-6	38
5			Oleic Acid	282	C18H34O2	000112-80-1	38



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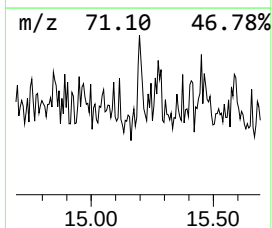
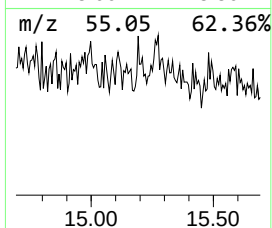
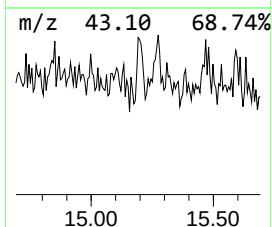
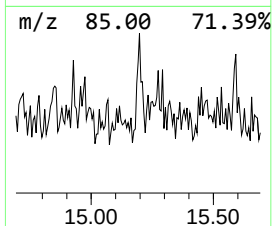
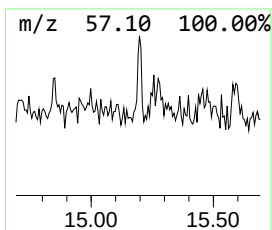
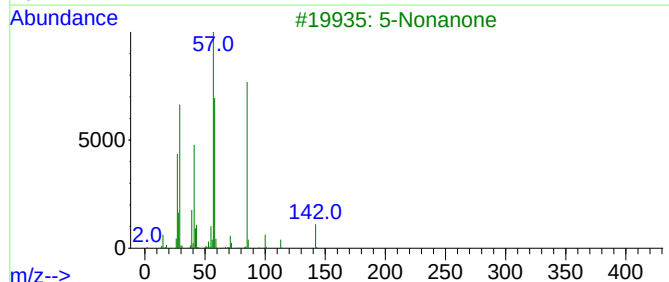
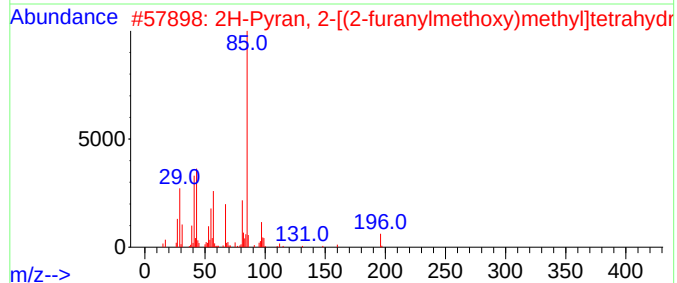
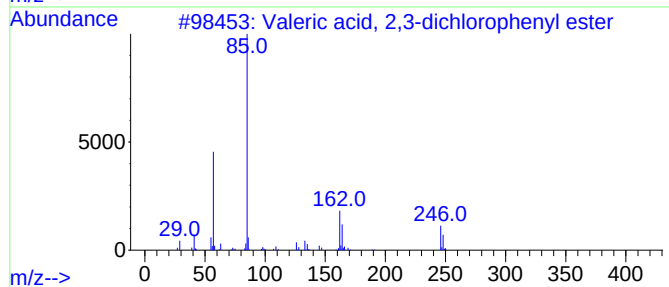
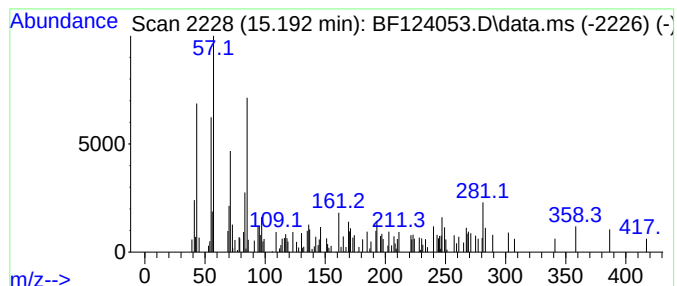
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.192 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	2.27 ng	38640	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Valeric acid, 2,3-dichlorophenyl...	246	C11H12Cl2O2	1000330-98-2	22
2			2H-Pyran, 2-[(2-furanylmethoxy)m...	196	C11H16O3	054845-37-3	18
3			5-Nonanone	142	C9H18O	000502-56-7	18
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	18
5			2-Butene, 1,4-diethoxy-	144	C8H16O2	007250-85-3	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124053.D
Acq On : 25 May 2021 19:29
Operator : JU/CG
Sample : M2502-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-052421

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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
Butane, 2-metho...	2.246	40.9	ng	926205	1	6.893	452983	20.0
Propane, 1,1-di...	2.352	2.4	ng	55072	1	6.893	452983	20.0
2-Pentanone, 4-...	5.128	27.3	ng	617329	1	6.893	452983	20.0
5-Eicosene, (E)-	13.927	17.9	ng	346430	5	14.069	386208	20.0
Hexanoic acid, ...	14.580	4.3	ng	83166	5	14.069	386208	20.0
unknown15.192	15.192	2.3	ng	38640	6	15.563	340352	20.0