

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052021\
 Data File : BF124005.D
 Acq On : 20 May 2021 12:47
 Operator : JU/CG
 Sample : PB136559BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136559BL

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: BF124005.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.304	27	37	44	rVB	71771	96288	3.97%	0.636%
2	2.410	49	55	60	rBB	23242	27954	1.15%	0.185%
3	4.057	330	335	340	rVB2	27088	32683	1.35%	0.216%
4	5.151	514	521	532	rBV	193142	265538	10.94%	1.754%
5	5.539	581	587	590	rBV	2085449	2071068	85.35%	13.677%
6	6.528	749	755	758	rBV	1723821	2037393	83.96%	13.455%
7	6.904	815	819	822	rBV	511467	392145	16.16%	2.590%
8	7.469	909	915	918	rBV	1366693	1385164	57.08%	9.148%
9	8.186	1032	1037	1041	rBV	563843	499238	20.57%	3.297%
10	9.269	1214	1221	1224	rBV	2461430	2426506	100.00%	16.025%
11	9.945	1331	1336	1339	rBV	711018	578340	23.83%	3.819%
12	10.733	1465	1470	1473	rBV	1663979	1466617	60.44%	9.685%
13	11.433	1585	1589	1592	rBV	620386	567149	23.37%	3.745%
14	13.021	1854	1859	1862	rBV	2761188	2334635	96.21%	15.418%
15	14.074	2029	2038	2041	rBV	456676	431370	17.78%	2.849%
16	15.492	2273	2279	2280	rBV3	17461	26925	1.11%	0.178%
17	15.568	2287	2292	2296	rBV	236400	304865	12.56%	2.013%
18	16.056	2370	2375	2380	rBV2	24685	41000	1.69%	0.271%
19	16.580	2459	2464	2470	rBV4	26771	45411	1.87%	0.300%
20	17.021	2529	2539	2541	rBV6	18839	42319	1.74%	0.279%
21	17.198	2562	2569	2576	rVB5	16335	39747	1.64%	0.262%
22	17.927	2687	2693	2701	rVB7	13167	30048	1.24%	0.198%

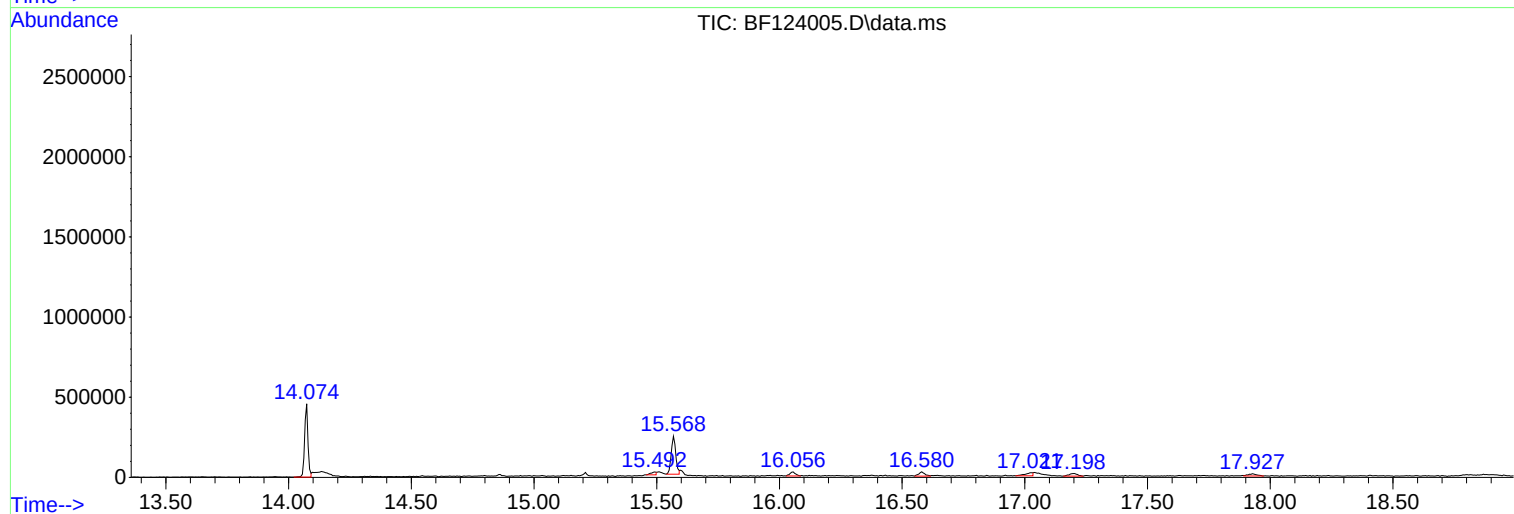
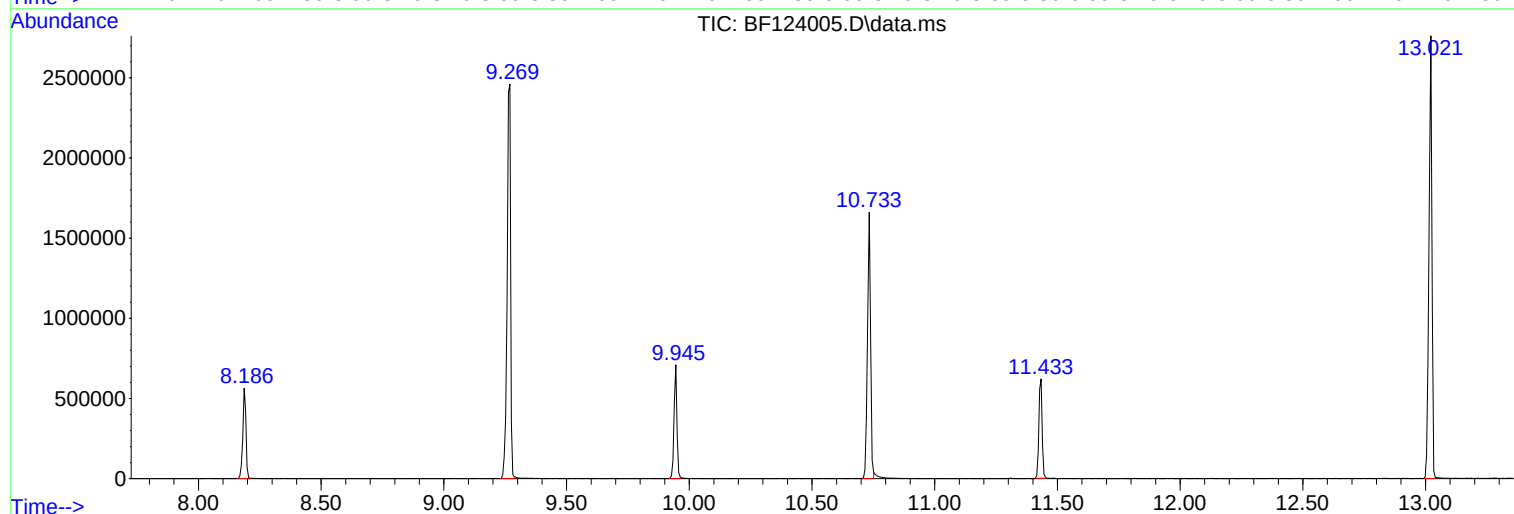
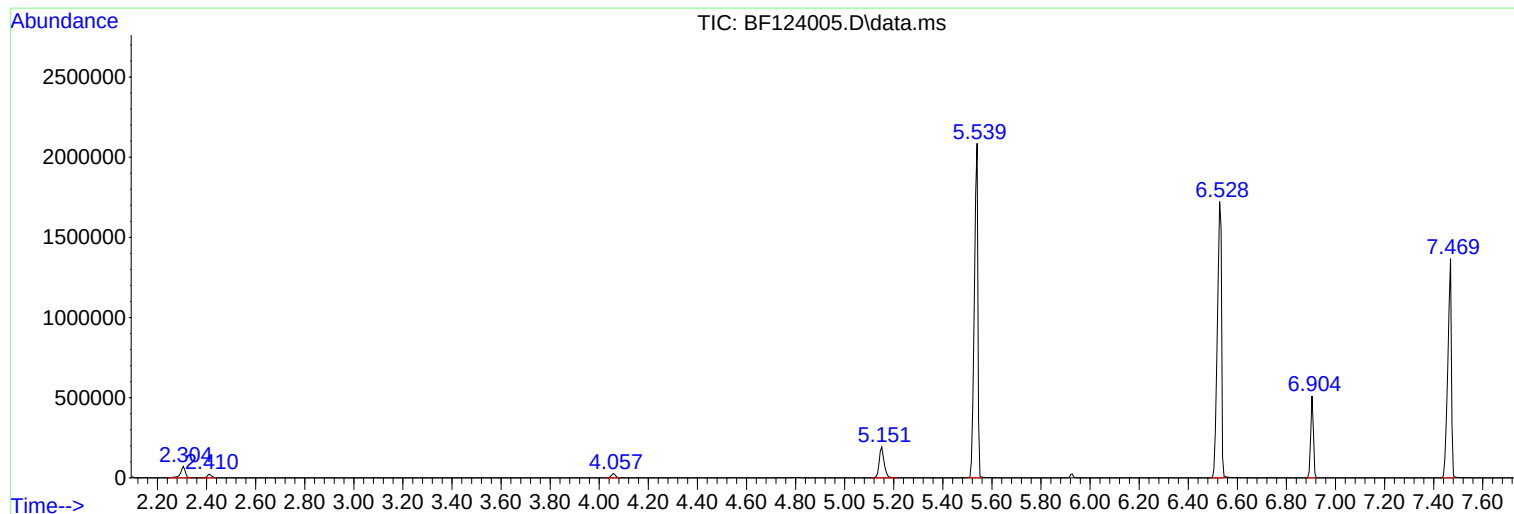
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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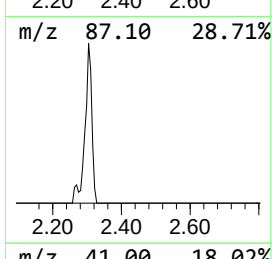
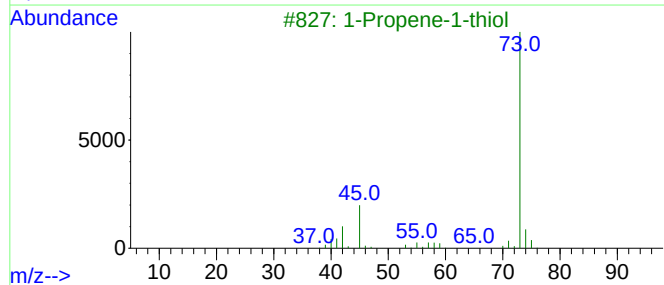
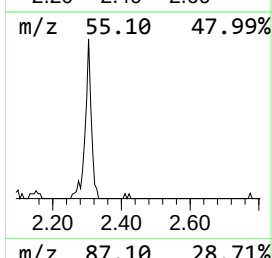
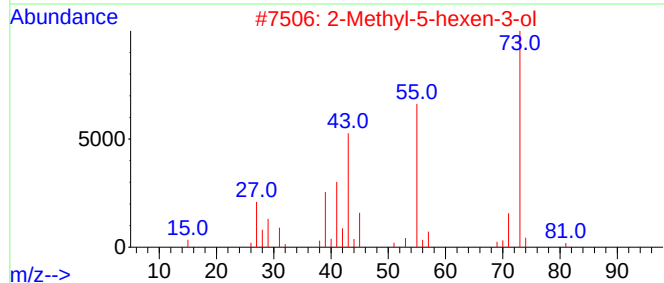
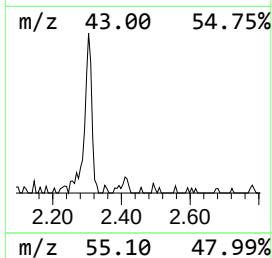
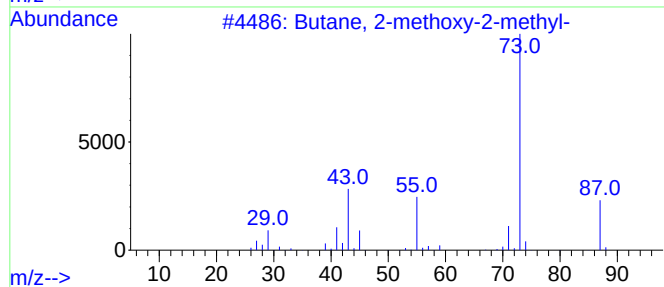
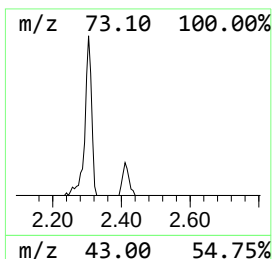
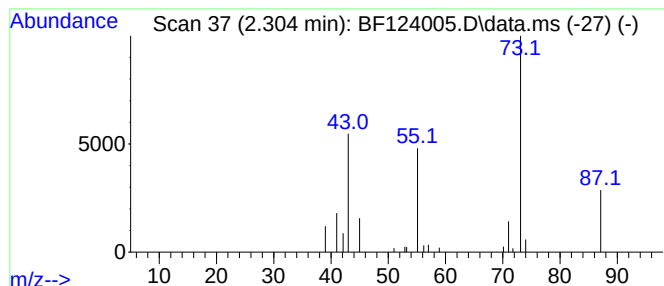
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.304	4.91 ng	96288	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	42
3			1-Propene-1-thiol	74	C3H6S	000925-89-3	27
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	17



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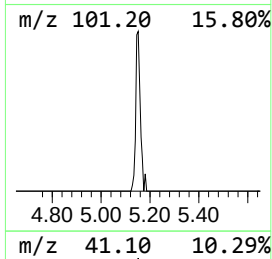
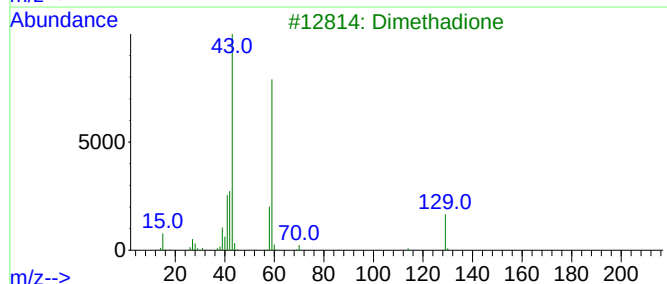
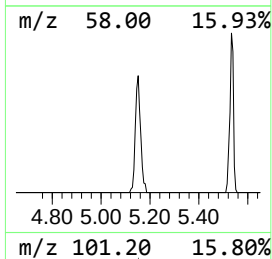
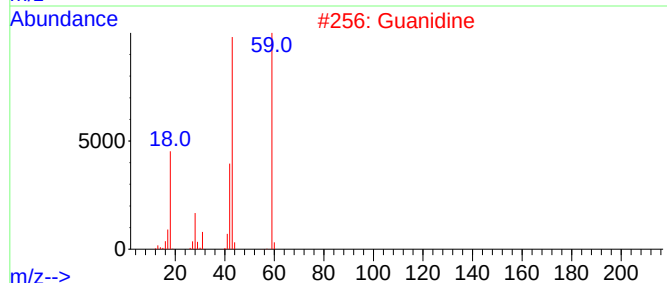
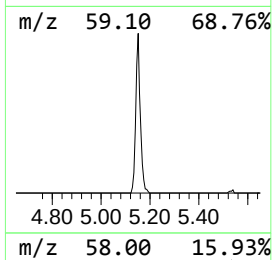
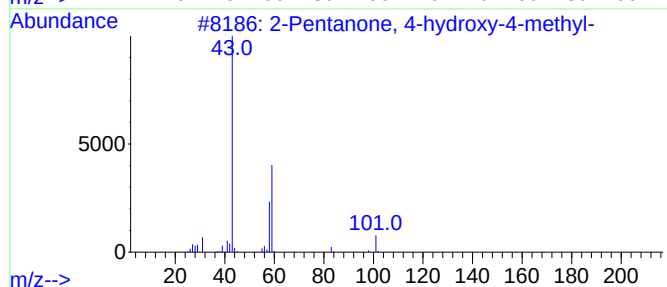
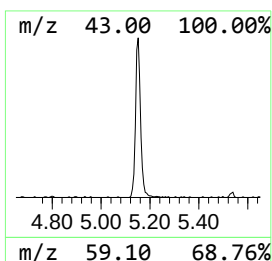
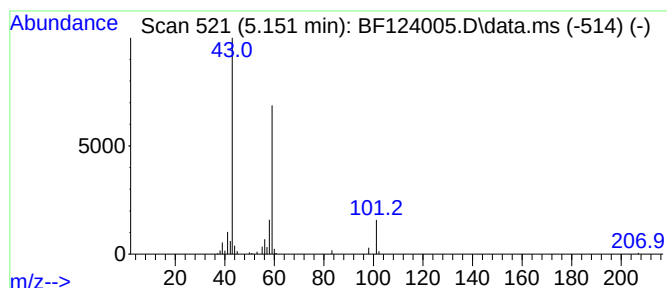
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	13.54 ng	265538	1,4-Dichlorobenzene-d4	6.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	56
2	Guanidine	59	CH5N3		000113-00-8	50
3	Dimethadione	129	C5H7NO3		000695-53-4	38
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	38
5	3-Octanol	130	C8H18O		000589-98-0	33



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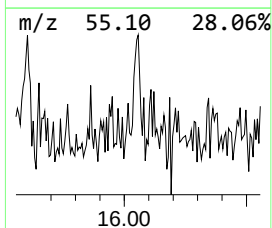
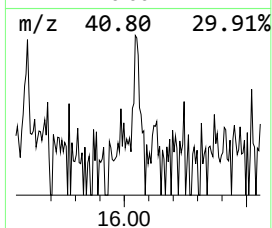
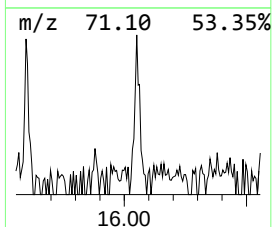
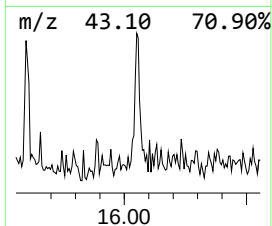
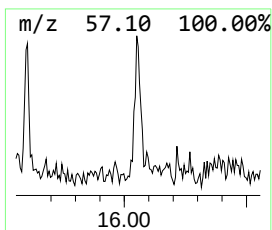
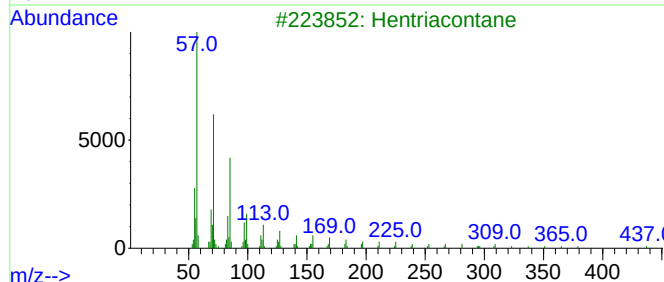
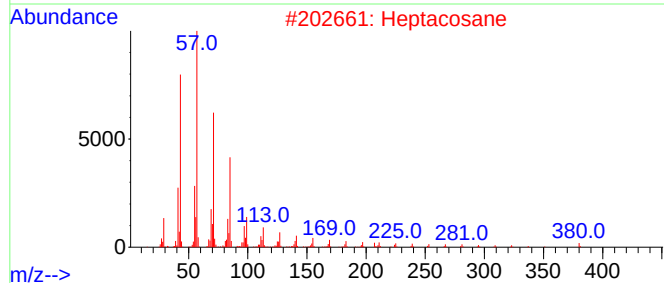
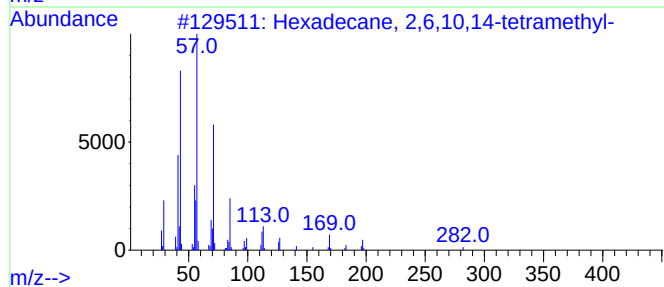
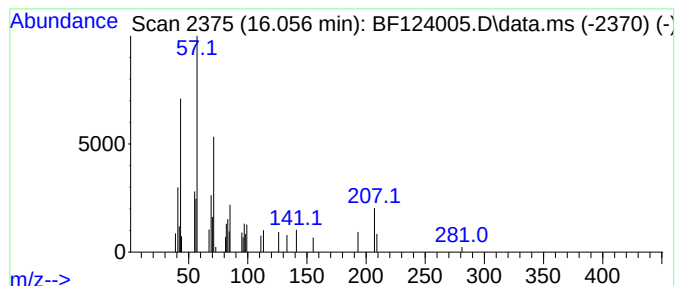
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown16.05 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.057	2.69 ng	41000	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	43
2			Heptacosane	380	C27H56	000593-49-7	43
3			Hentriacontane	437	C31H64	000630-04-6	43
4			2,3-Dimethyldecane	170	C12H26	017312-44-6	43
5			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	43



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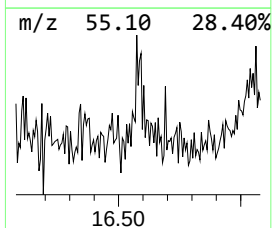
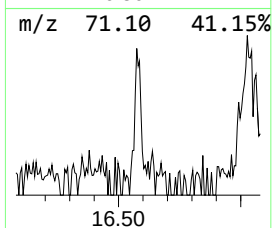
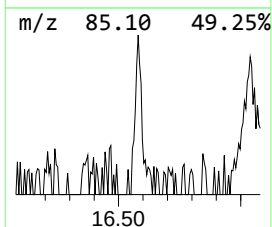
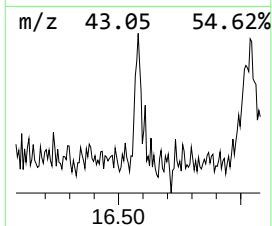
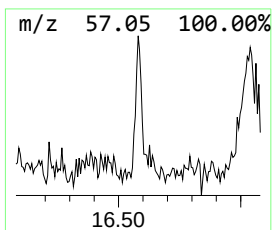
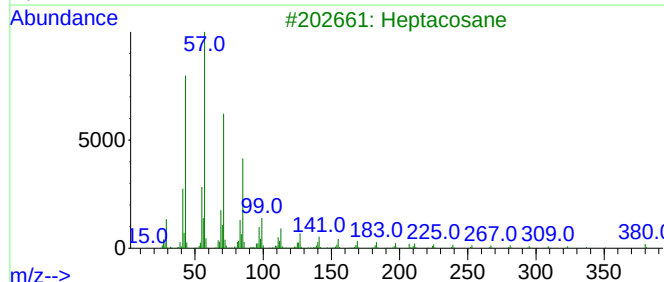
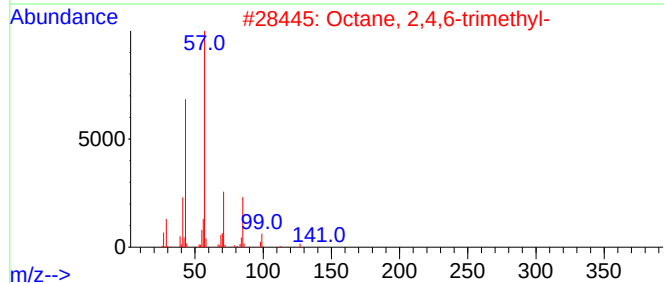
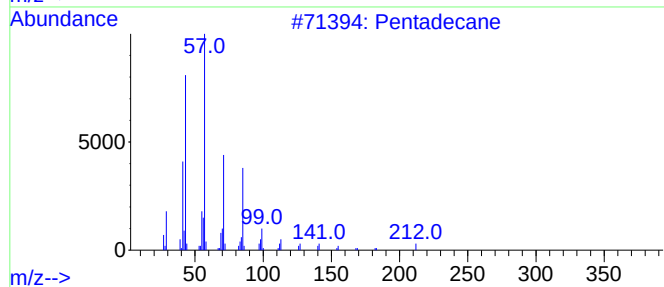
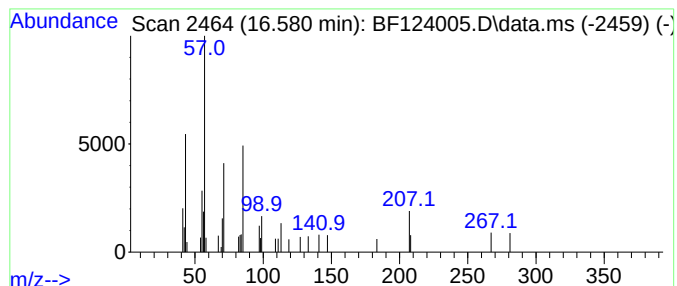
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Peak Number 4 Pentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.580	2.98 ng	45411	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	53
2			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	50
3			Heptacosane	380	C27H56	000593-49-7	50
4			Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	47
5			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	43



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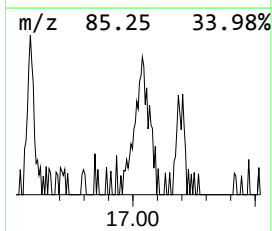
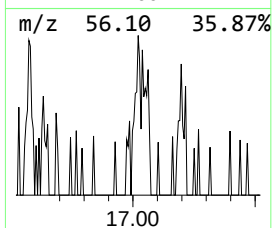
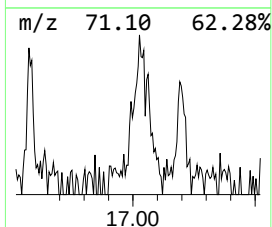
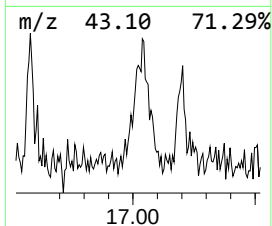
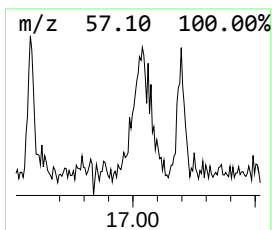
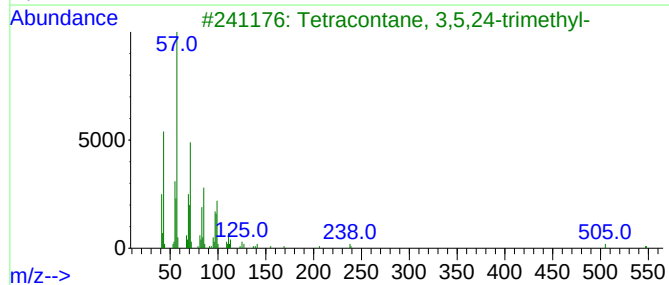
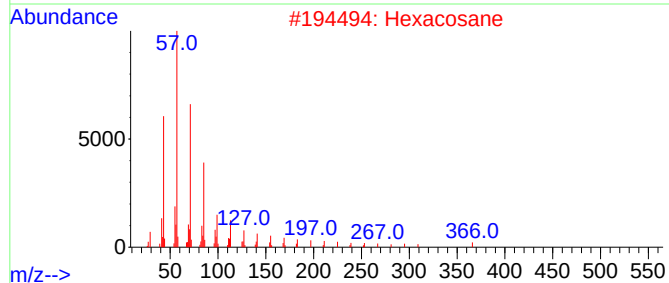
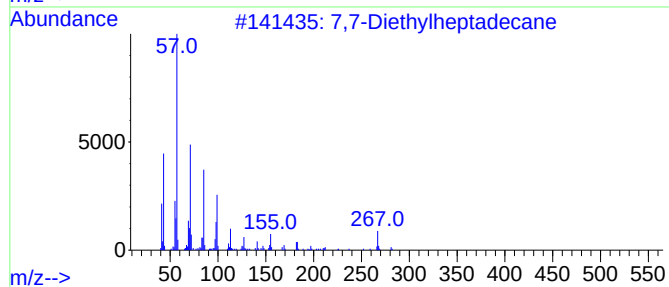
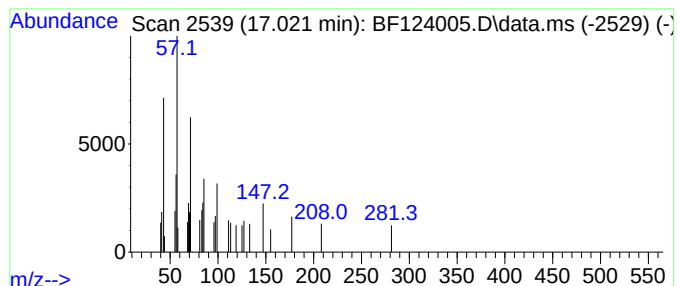
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown17.02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.021	2.78 ng	42319	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,7-Diethylheptadecane			296	C21H44	1000360-41-5	43
2	Hexacosane			366	C26H54	000630-01-3	38
3	Tetracontane, 3,5,24-trimethyl-			605	C43H88	055162-61-3	38
4	1-Octadecanesulphonyl chloride			352	C18H37ClO2S	1000342-70-4	38
5	Hexadecane, 1-chloro-			260	C16H33Cl	004860-03-1	35



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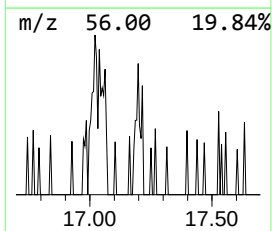
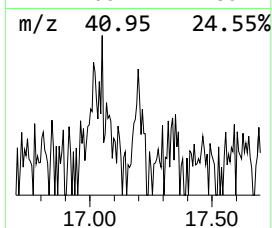
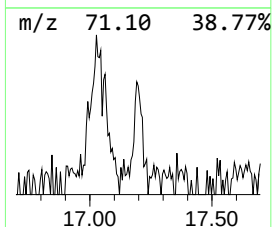
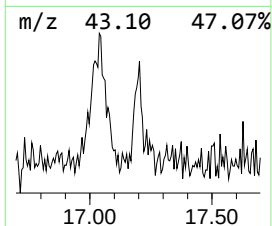
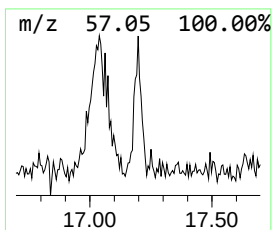
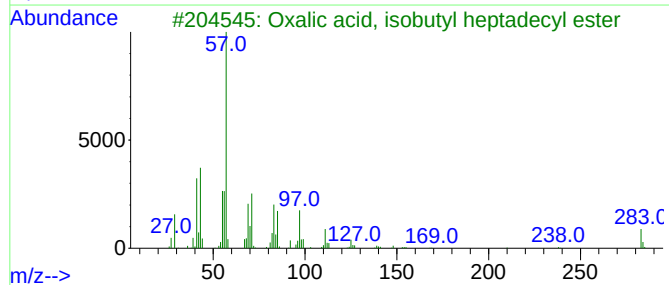
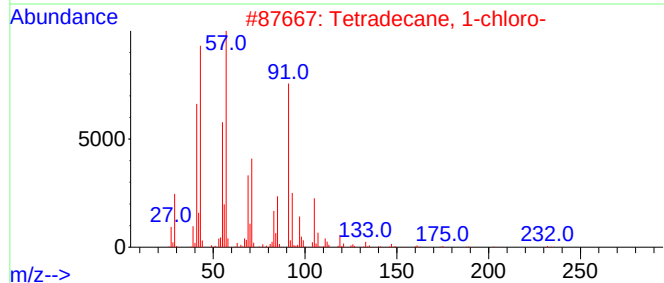
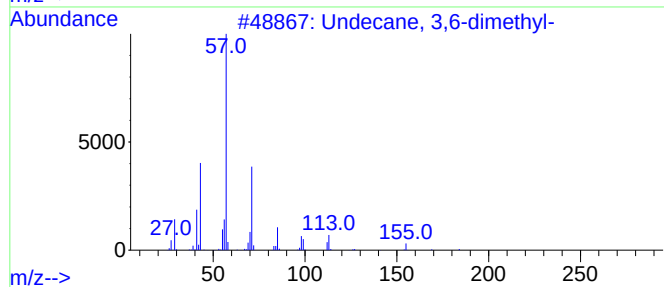
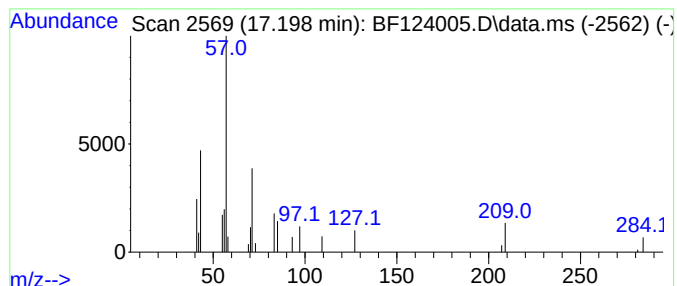
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Undecane, 3,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.198	2.61 ng	39747	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	53
2			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	50
3			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	43
4			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1000309-37-4	43
5			Dichloroacetic acid, 2-octyl ester	240	C10H18Cl2O2	096980-53-9	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052021\
Data File : BF124005.D
Acq On : 20 May 2021 12:47
Operator : JU/CG
Sample : PB136559BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136559BL

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...	2.304	4.9	ng	96288	1	6.904	392145	20.0
2-Pentanone, 4-...	5.151	13.5	ng	265538	1	6.904	392145	20.0
unknown16.05	16.057	2.7	ng	41000	6	15.568	304865	20.0
Pentadecane	16.580	3.0	ng	45411	6	15.568	304865	20.0
unknown17.02	17.021	2.8	ng	42319	6	15.568	304865	20.0
Undecane, 3,6-d...	17.198	2.6	ng	39747	6	15.568	304865	20.0