

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
 Data File : BF123632.D
 Acq On : 19 Apr 2021 20:27
 Operator : JU/CG
 Sample : M2063-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP2-0-2

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-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123632.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	13	rVB	1543043	1860555	30.84%	4.125%
2	5.081	504	509	515	rVB	57349	71456	1.18%	0.158%
3	5.487	574	578	582	rBV	6805040	5869259	97.29%	13.013%
4	6.498	746	750	753	rBV	6663678	6032913	100.00%	13.376%
5	6.863	808	812	815	rBV	1873840	1408027	23.34%	3.122%
6	7.422	902	907	910	rBV	4184073	4027644	66.76%	8.930%
7	8.145	1026	1030	1034	rBV	2122840	1752945	29.06%	3.887%
8	9.228	1209	1214	1217	rBV	6964115	5684938	94.23%	12.604%
9	9.616	1277	1280	1284	rBV	342692	266055	4.41%	0.590%
10	9.904	1326	1329	1333	rVB	2021623	1668975	27.66%	3.700%
11	10.692	1459	1463	1467	rBV	3492718	3330348	55.20%	7.384%
12	11.392	1578	1582	1585	rBV	1702433	1504408	24.94%	3.335%
13	11.416	1585	1586	1589	rVB	373265	228114	3.78%	0.506%
14	11.898	1664	1668	1670	rBV	106652	100097	1.66%	0.222%
15	11.922	1670	1672	1677	rVB	297572	250015	4.14%	0.554%
16	12.004	1683	1686	1689	rBV2	113419	111771	1.85%	0.248%
17	12.445	1757	1761	1764	rBV	108905	112273	1.86%	0.249%
18	12.610	1785	1789	1792	rVB	452613	365124	6.05%	0.810%
19	12.839	1823	1828	1830	rBV	498870	445387	7.38%	0.987%
20	12.986	1849	1853	1856	rBV	4789307	4005851	66.40%	8.882%
21	13.057	1861	1865	1873	rBV6	58962	103178	1.71%	0.229%
22	13.168	1882	1884	1887	rVB	83024	68857	1.14%	0.153%
23	13.233	1890	1895	1898	rVV4	52391	74878	1.24%	0.166%
24	13.268	1898	1901	1904	rVB2	78343	82946	1.37%	0.184%
25	13.674	1968	1970	1975	rVB2	77739	78566	1.30%	0.174%
26	13.780	1984	1988	1992	rBV4	57483	106537	1.77%	0.236%
27	13.915	2002	2011	2025	rBV6	196011	654846	10.85%	1.452%
28	14.039	2027	2032	2035	rVV	1513940	1620065	26.85%	3.592%
29	14.063	2035	2036	2044	rVB	270010	220137	3.65%	0.488%
30	14.515	2110	2113	2116	rVB3	94999	91760	1.52%	0.203%
31	14.551	2116	2119	2121	rBV4	68618	78433	1.30%	0.174%
32	14.904	2176	2179	2182	rBV3	52161	67765	1.12%	0.150%
33	14.974	2188	2191	2198	rBV2	134850	164860	2.73%	0.366%
34	15.086	2206	2210	2213	rBV	197672	275936	4.57%	0.612%
35	15.174	2221	2225	2227	rBV2	95082	117534	1.95%	0.261%
36	15.392	2259	2262	2268	rVB	149105	202280	3.35%	0.448%

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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-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.457	2269	2273	2277	rBV	175021	214141	3.55%	0.475%
38	15.521	2279	2284	2288	rBV2	1020798	1286588	21.33%	2.853%
39	15.762	2323	2325	2331	rVB5	77335	98061	1.63%	0.217%
40	16.009	2362	2367	2371	rBV	124655	193605	3.21%	0.429%
41	17.004	2532	2536	2543	rVB2	69839	138614	2.30%	0.307%
42	17.133	2556	2558	2563	rVB5	53299	67492	1.12%	0.150%

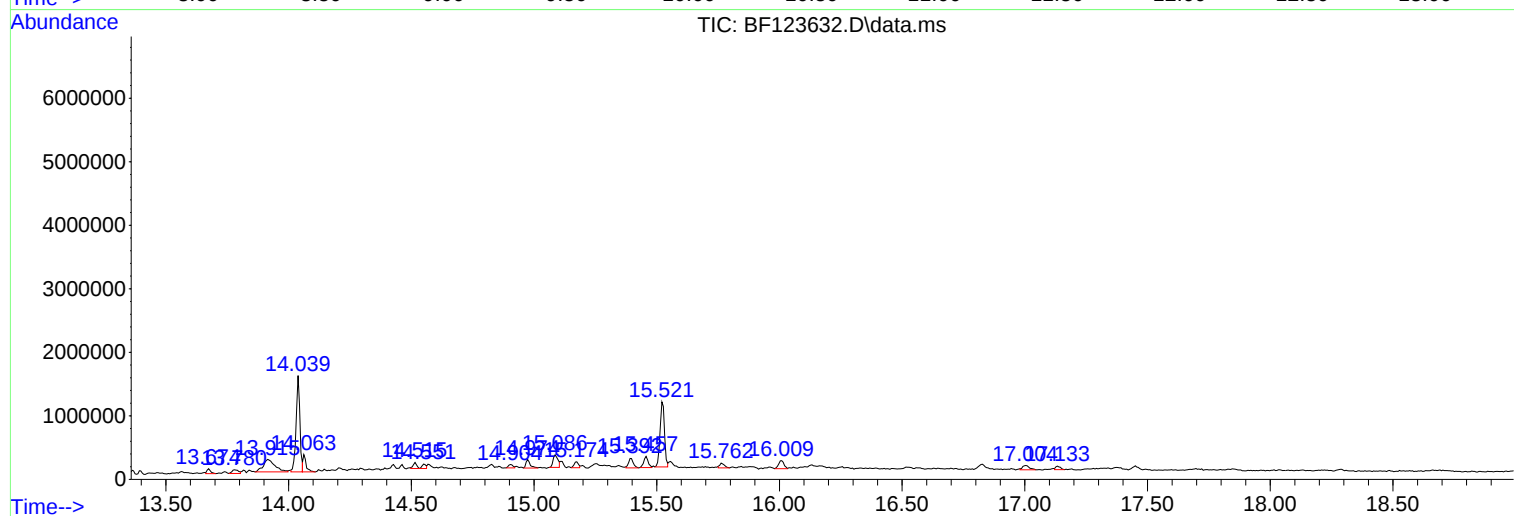
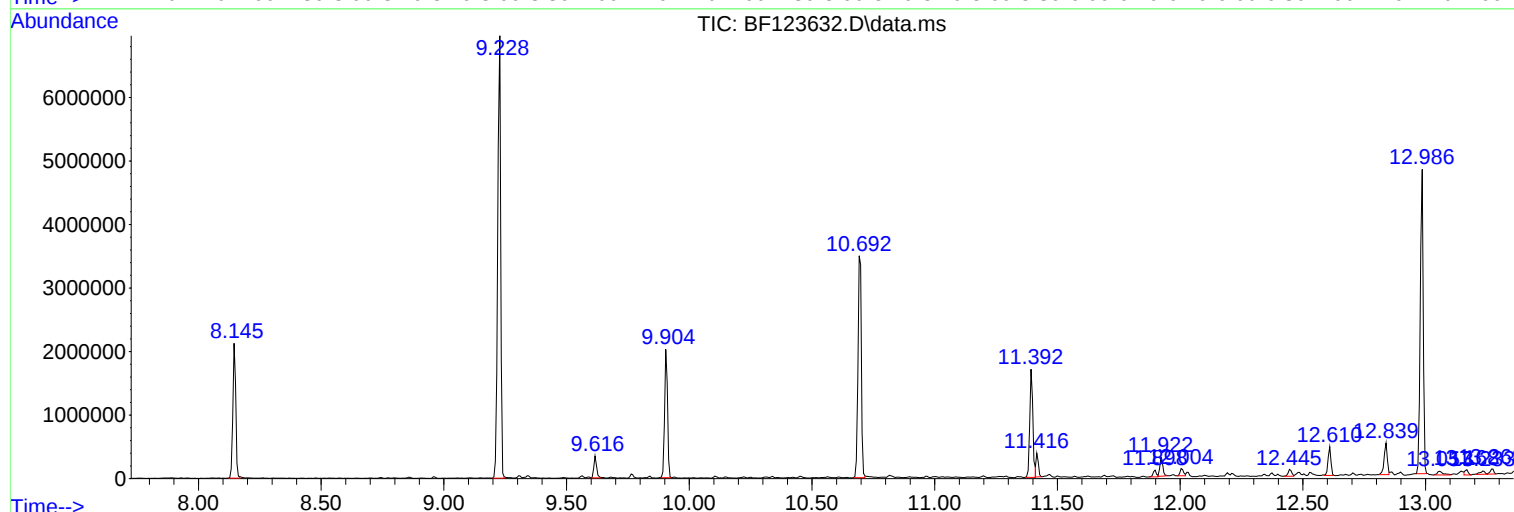
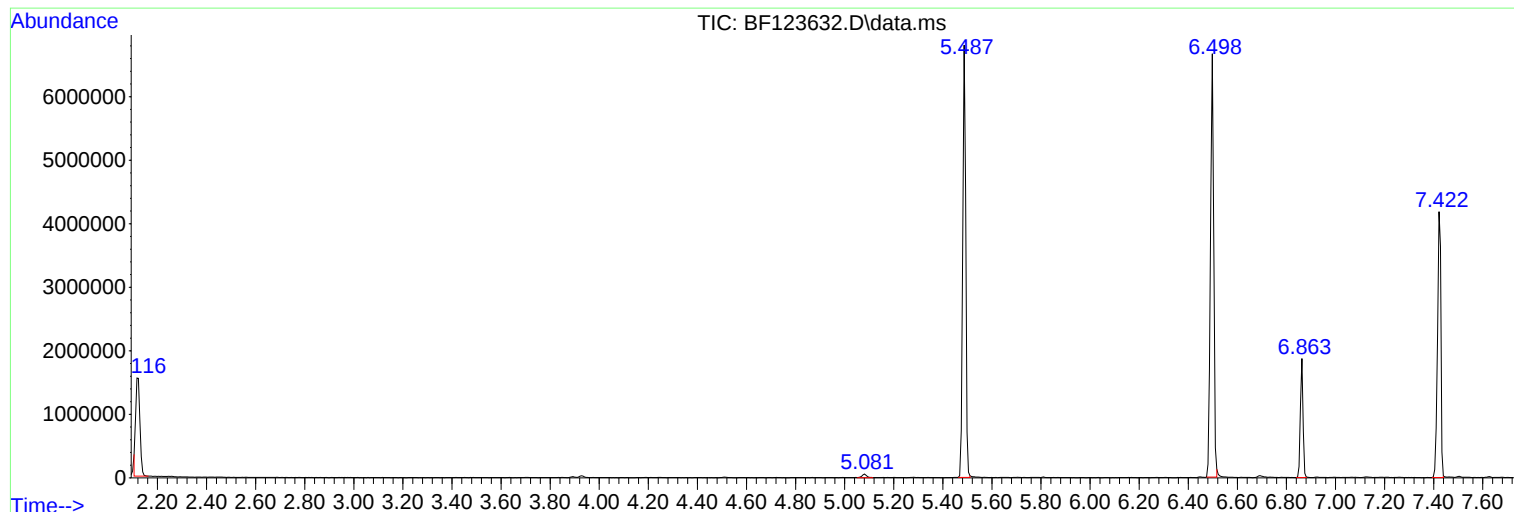
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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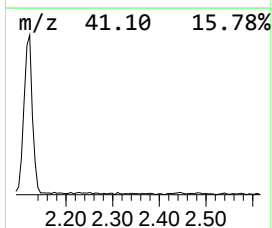
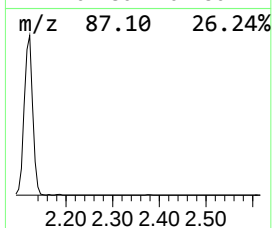
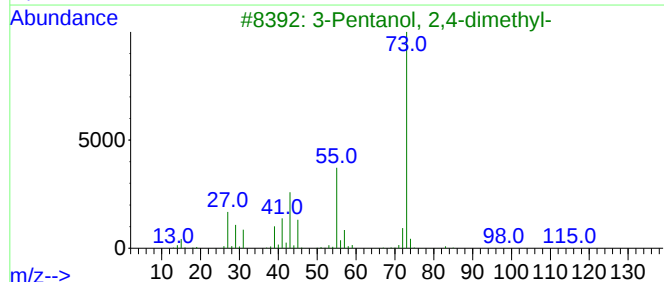
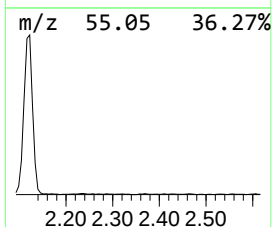
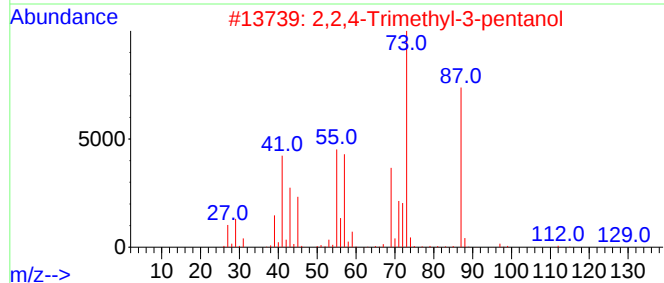
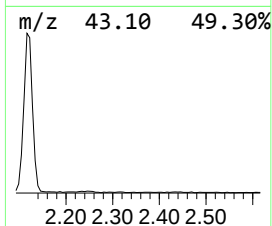
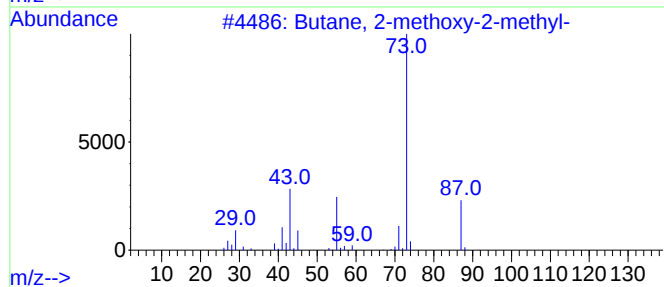
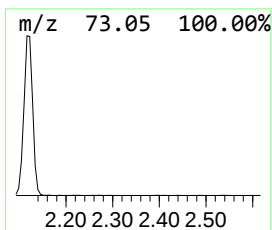
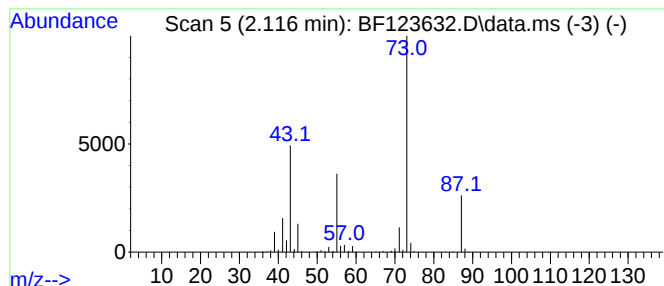
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.116	26.43 ng	1860560	1,4-Dichlorobenzene-d4	6.863

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	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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Instrument :
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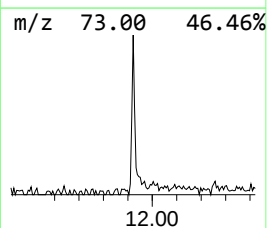
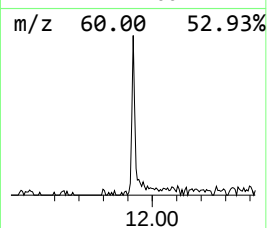
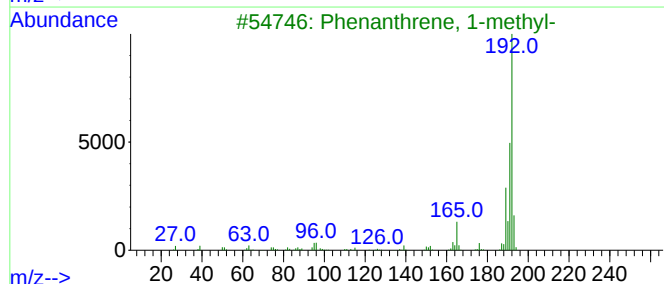
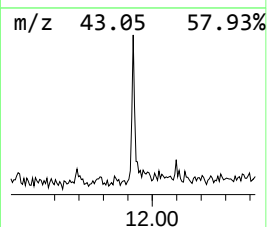
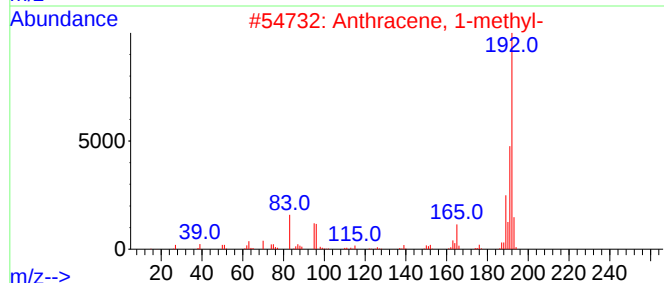
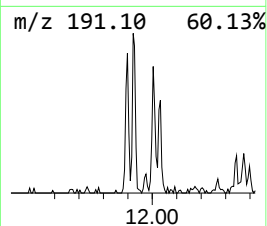
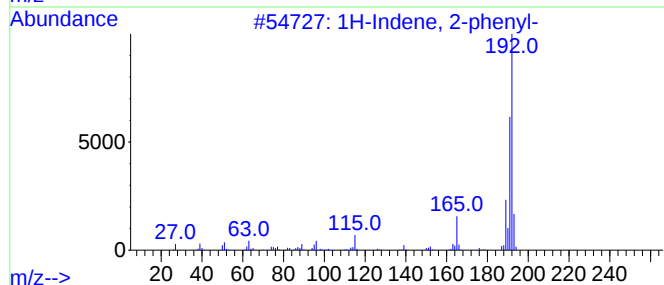
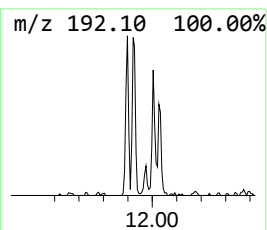
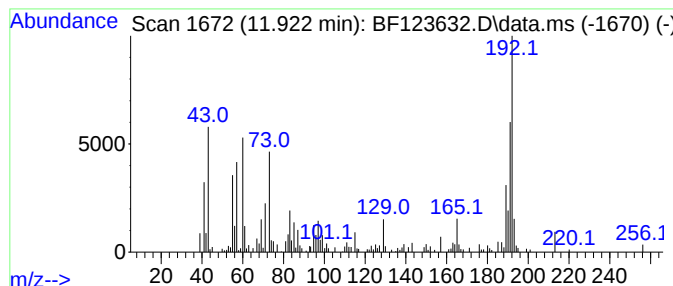
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1H-Indene, 2-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.32 ng	250015	Phenanthrene-d10	11.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	92
2		Anthracene, 1-methyl-	192	C15H12	000610-48-0	78
3		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	78
4		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	78
5		Anthracene, 2-methyl-	192	C15H12	000613-12-7	70



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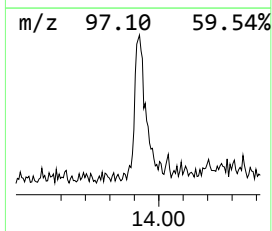
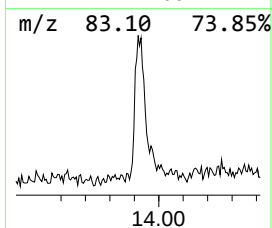
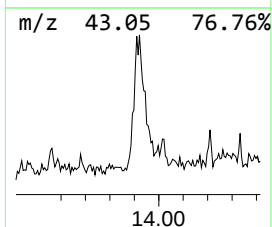
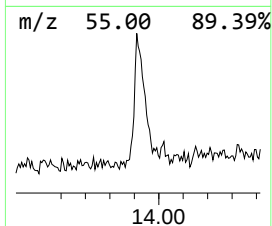
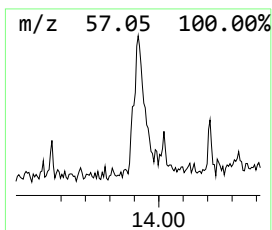
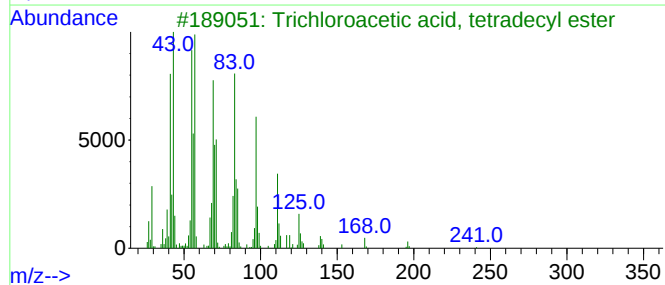
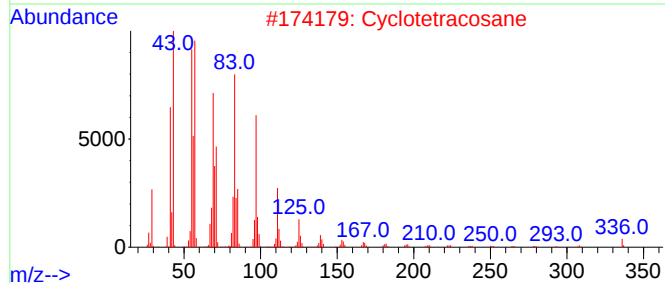
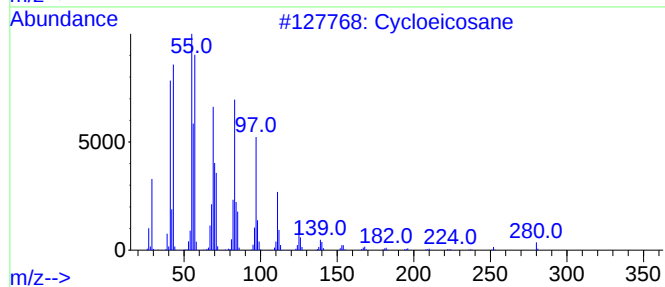
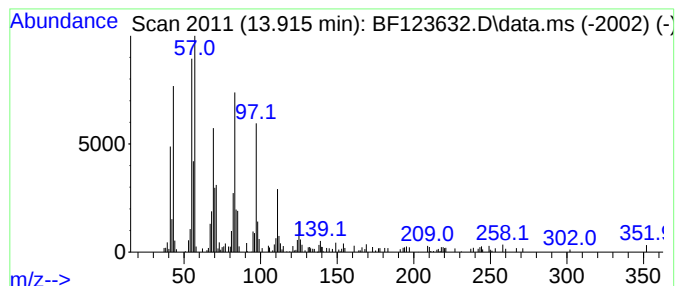
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cycloeicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	8.08 ng	654846	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	91
2			Cyclotetracosane	336	C24H48	000297-03-0	90
3			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
4			1-Heneicosanol	312	C21H44O	015594-90-8	87
5			11-Tricosene	322	C23H46	052078-56-5	87



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Instrument :
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ClientSampled :
TP2-0-2

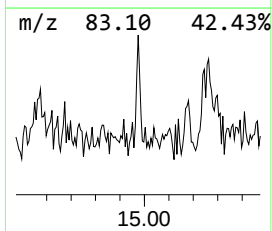
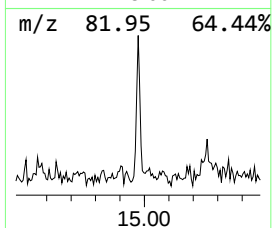
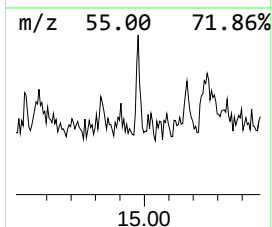
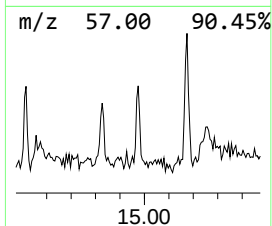
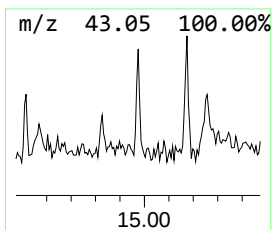
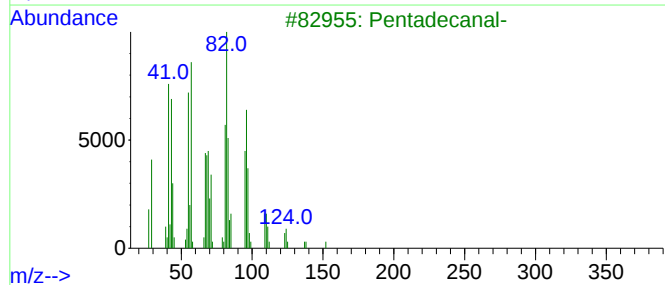
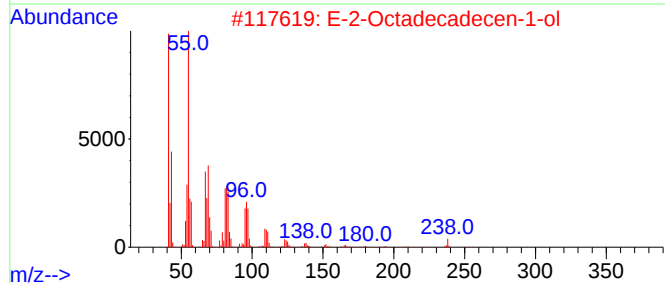
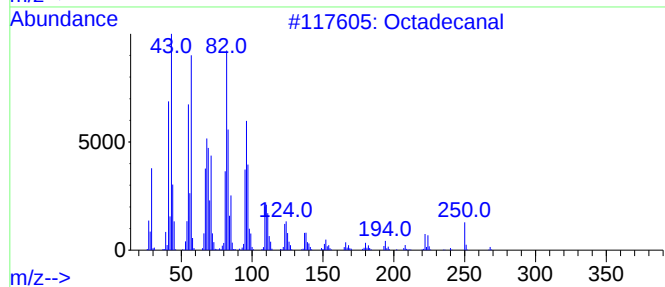
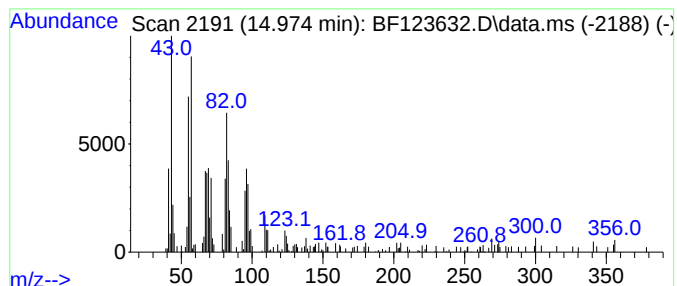
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	2.56 ng	164860	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	90
2			E-2-Octadecadecen-1-ol	268	C18H36O	1000131-10-2	81
3			Pentadecanal-	226	C15H30O	002765-11-9	81
4			1,13-Tetradecadiene	194	C14H26	021964-49-8	78
5			Heptadecanal	254	C17H34O	1000376-70-0	74



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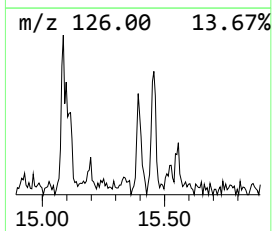
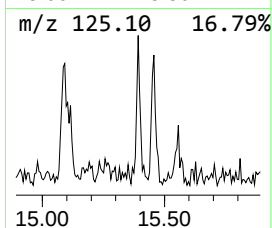
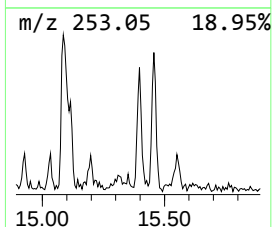
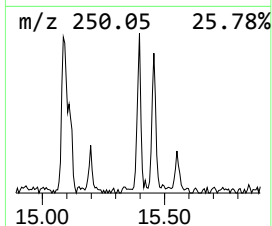
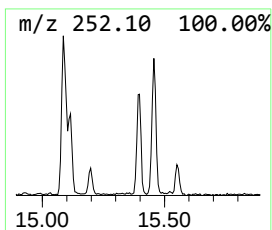
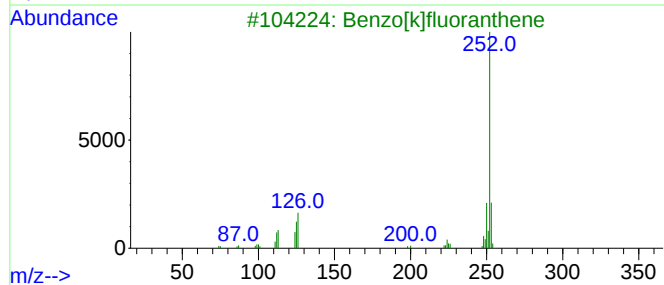
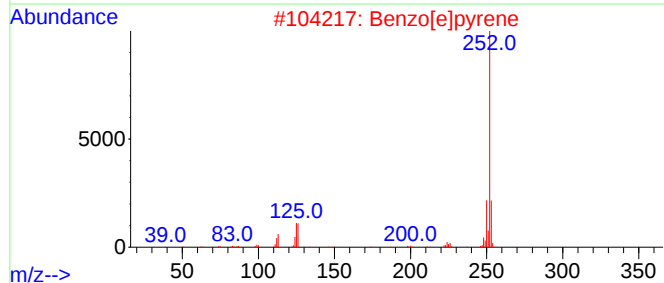
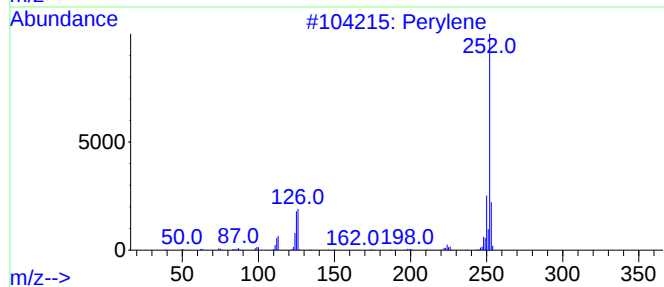
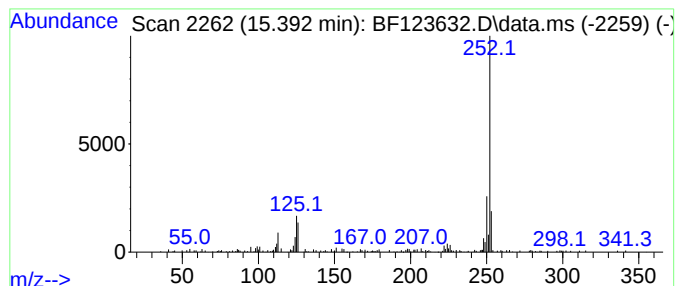
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	3.14 ng	202280	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	93
2			Benzo[e]pyrene	252	C20H12	000192-97-2	91
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
4			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	91
5			Benzo[a]pyrene	252	C20H12	000050-32-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123632.D
Acq On : 19 Apr 2021 20:27
Operator : JU/CG
Sample : M2063-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2-0-2

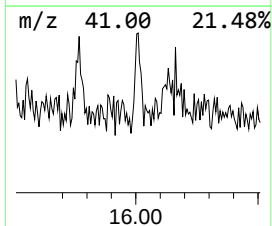
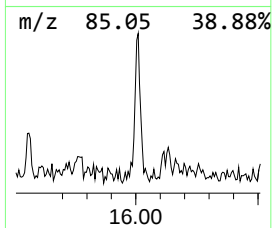
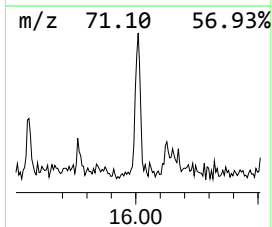
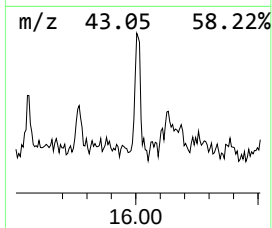
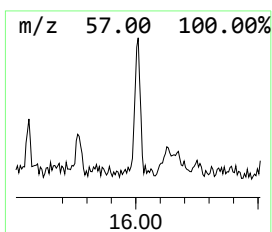
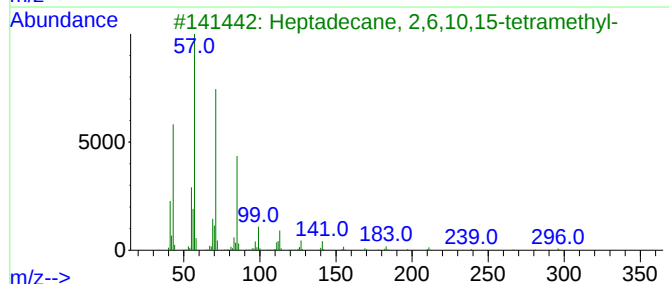
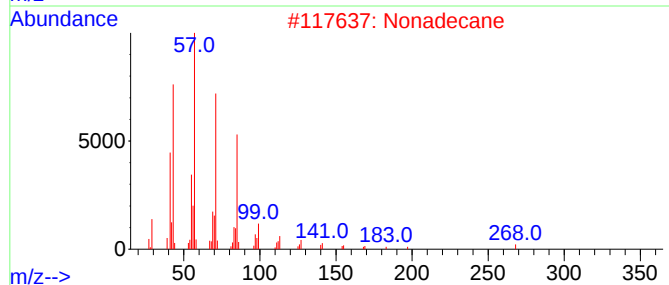
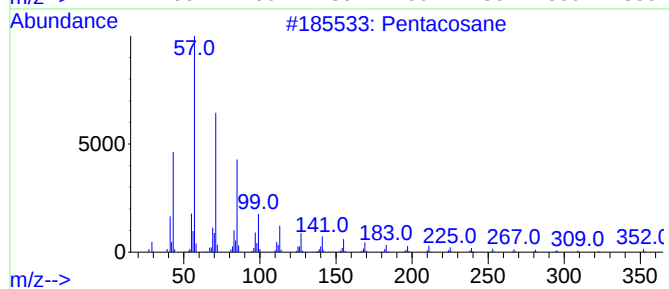
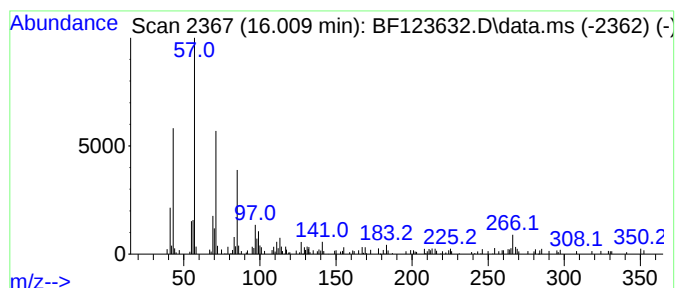
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	3.01 ng	193605	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	93
2			Nonadecane	268	C19H40	000629-92-5	93
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
4			Pentadecane	212	C15H32	000629-62-9	90
5			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123632.D
Acq On : 19 Apr 2021 20:27
Operator : JU/CG
Sample : M2063-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2-0-2

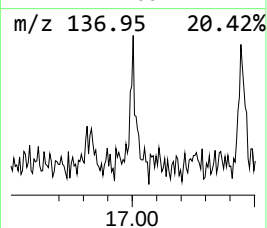
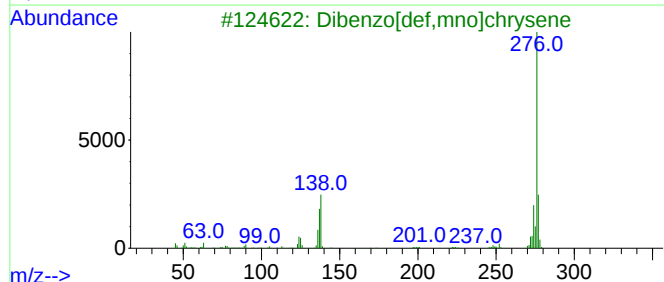
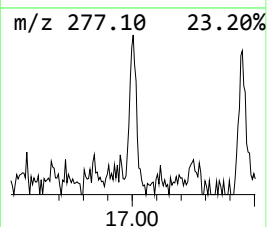
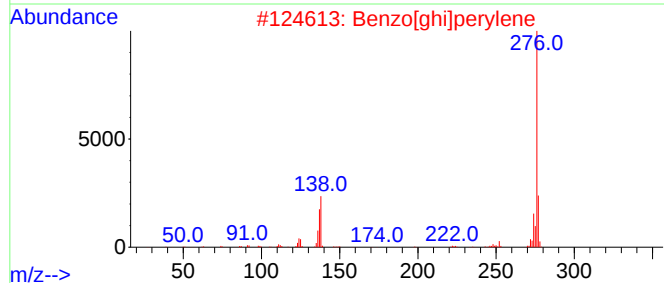
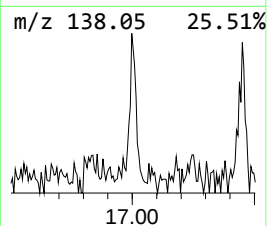
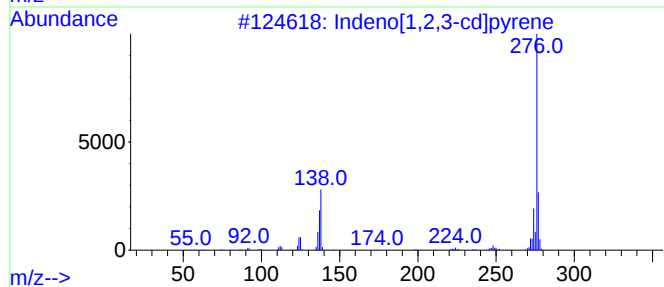
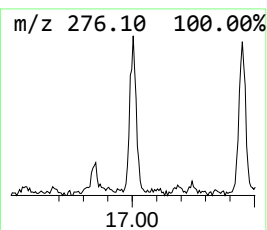
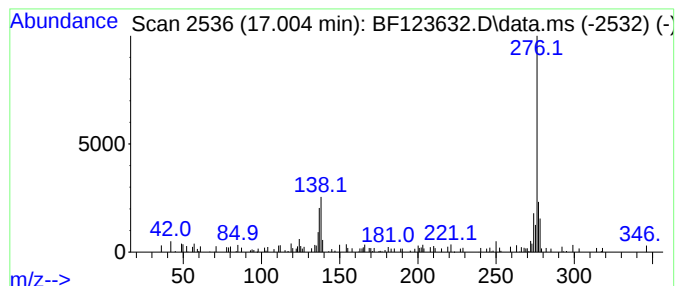
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dibenzo[def,mno]chrysene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.003	2.15 ng	138614	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	93
2			Benzo[ghi]perylene	276	C22H12	000191-24-2	91
3			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	91
4			Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	87
5			2-Amino-3-cyano-4,5-diphenylthio...	276	C17H12N2S	042160-34-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123632.D
Acq On : 19 Apr 2021 20:27
Operator : JU/CG
Sample : M2063-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2-0-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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...	2.116	26.4	ng	1860560	1	6.863	1408030	20.0
1H-Indene, 2-ph...	11.922	3.3	ng	250015	4	11.392	1504410	20.0
Cycloeicosane	13.916	8.1	ng	654846	5	14.039	1620070	20.0
Octadecanal	14.974	2.6	ng	164860	6	15.521	1286590	20.0
Perylene	15.392	3.1	ng	202280	6	15.521	1286590	20.0
Pentacosane	16.009	3.0	ng	193605	6	15.521	1286590	20.0
Dibenzo[def,mno...	17.003	2.1	ng	138614	6	15.521	1286590	20.0