

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030222\
 Data File : BF127152.D
 Acq On : 02 Mar 2022 17:39
 Operator : CG\JU
 Sample : N1721-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUM-4

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127152.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.116	476	481	486	rBV	114799	134442	5.57%	0.803%
2	5.510	544	548	552	rBV	2155174	2154399	89.20%	12.868%
3	6.516	714	719	731	rBV	2097945	2252840	93.28%	13.456%
4	6.887	779	782	786	rBV	652788	513772	21.27%	3.069%
5	7.451	873	878	881	rBV	1524437	1482937	61.40%	8.857%
6	8.069	979	983	993	rBV	70194	88750	3.67%	0.530%
7	8.169	996	1000	1004	rBV	775124	696541	28.84%	4.160%
8	9.251	1178	1184	1187	rBV	2581326	2415115	100.00%	14.425%
9	9.928	1296	1299	1303	rBV	852359	747772	30.96%	4.466%
10	10.722	1430	1434	1437	rBV	1818930	1500324	62.12%	8.961%
11	11.422	1549	1553	1555	rBV	823987	711175	29.45%	4.248%
12	11.445	1555	1557	1560	rVB	151628	119953	4.97%	0.716%
13	11.798	1614	1617	1621	rVB	45434	39605	1.64%	0.237%
14	12.033	1653	1657	1660	rBV2	24568	25775	1.07%	0.154%
15	12.633	1755	1759	1763	rBV	239009	202432	8.38%	1.209%
16	12.863	1792	1798	1801	rBV	179066	182436	7.55%	1.090%
17	13.004	1818	1822	1826	rVB	1959786	1657362	68.62%	9.899%
18	13.927	1972	1979	1991	rVB10	28934	93452	3.87%	0.558%
19	14.063	1998	2002	2005	rBV	420400	418959	17.35%	2.502%
20	14.092	2005	2007	2012	rVB	61918	55860	2.31%	0.334%
21	14.574	2082	2089	2091	rBV8	21751	32951	1.36%	0.197%
22	15.116	2177	2181	2185	rBV	66602	111615	4.62%	0.667%
23	15.174	2188	2191	2196	rVB	60570	66058	2.74%	0.395%
24	15.427	2230	2234	2241	rVB	41867	53613	2.22%	0.320%
25	15.492	2241	2245	2251	rVB	57686	74584	3.09%	0.445%
26	15.557	2251	2256	2267	rBV2	384300	485650	20.11%	2.901%
27	15.774	2289	2293	2301	rVB4	30607	48760	2.02%	0.291%
28	16.010	2329	2333	2339	rVB	36238	56720	2.35%	0.339%
29	16.839	2469	2474	2479	rBV5	23262	43578	1.80%	0.260%
30	17.062	2508	2512	2519	rVB2	25129	46458	1.92%	0.277%
31	17.521	2586	2590	2597	rVB3	22939	44516	1.84%	0.266%
32	18.245	2707	2713	2732	rVB3	46908	184011	7.62%	1.099%

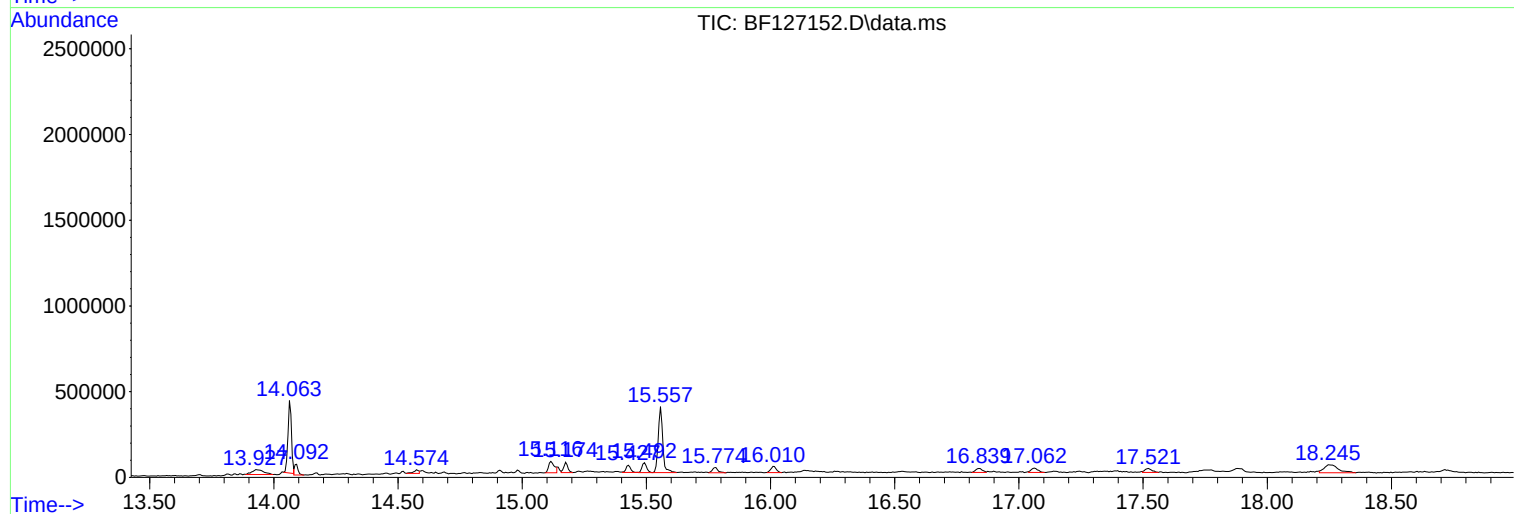
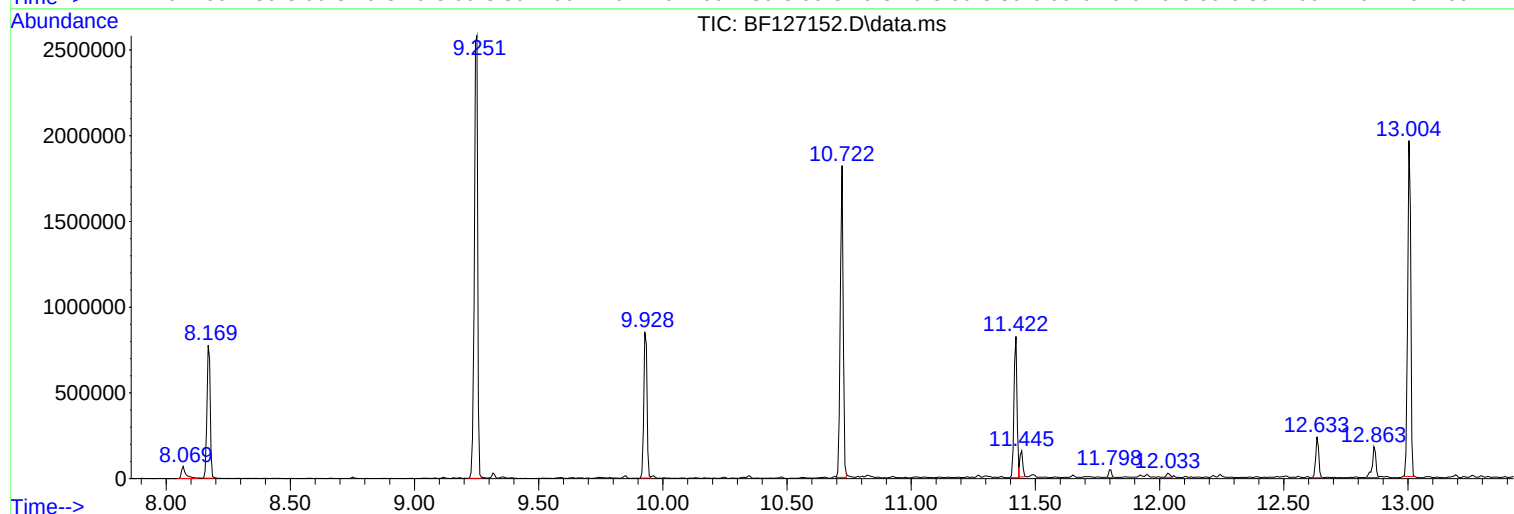
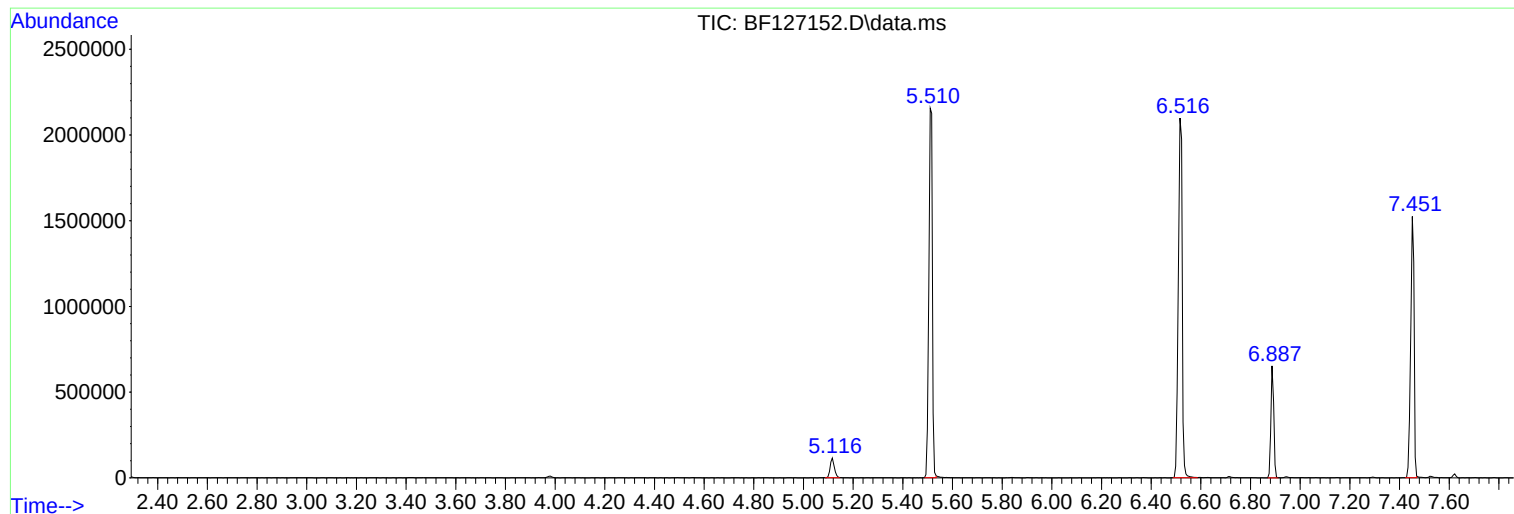
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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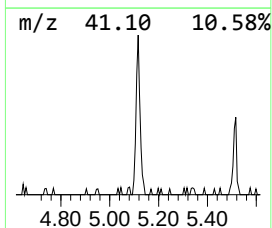
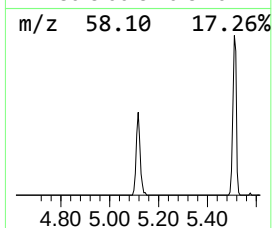
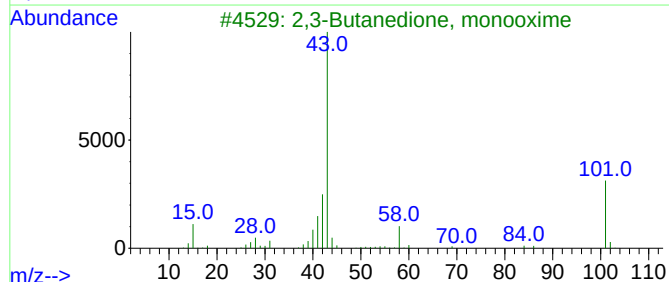
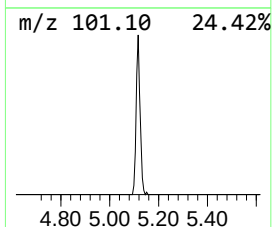
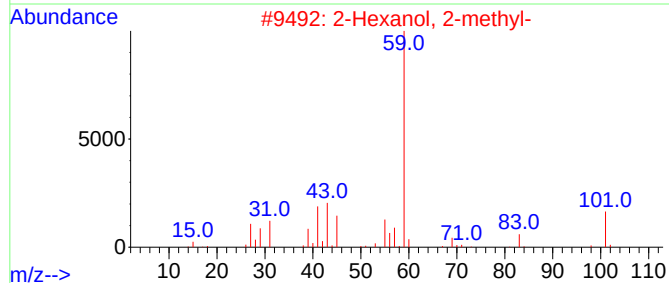
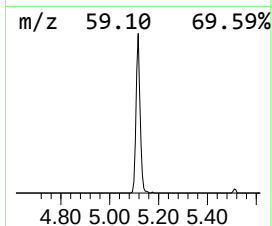
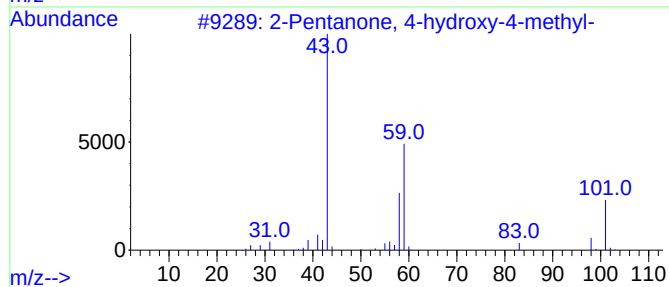
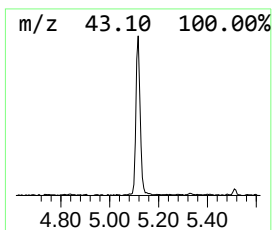
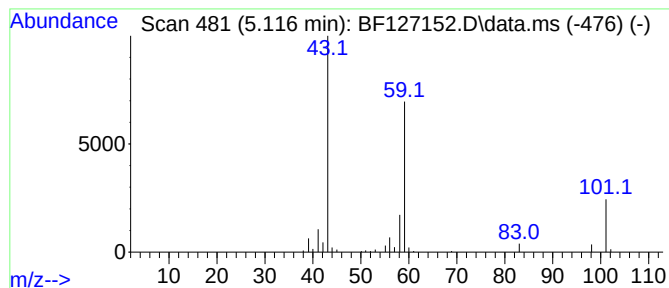
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	5.23 ng	134442	1,4-Dichlorobenzene-d4	6.887

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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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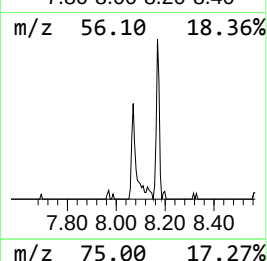
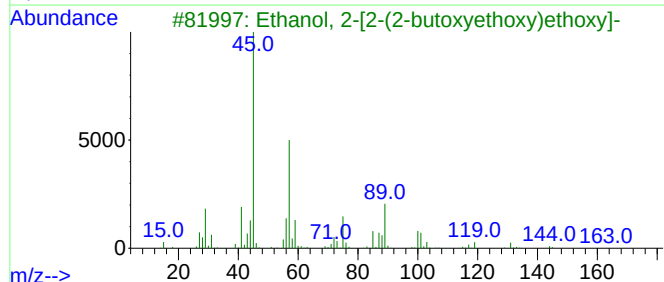
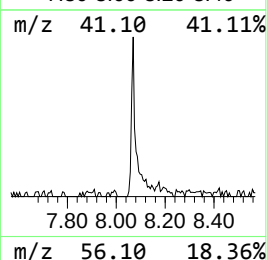
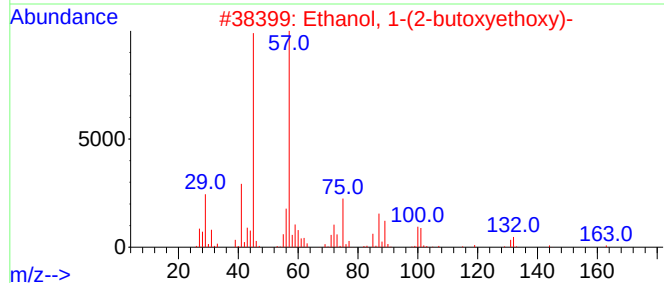
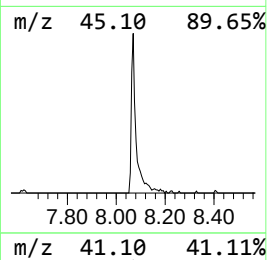
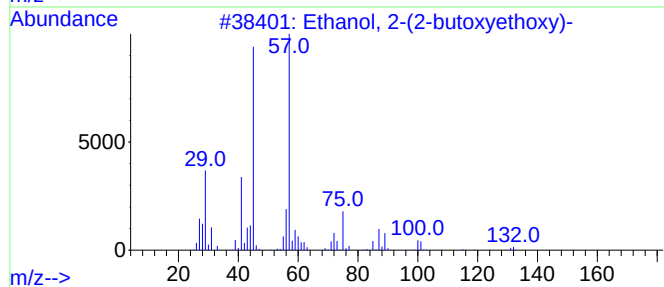
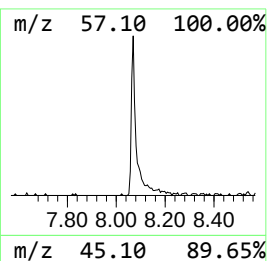
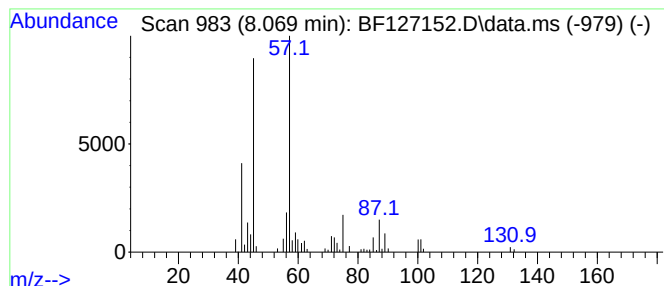
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	2.55 ng	88750	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	53



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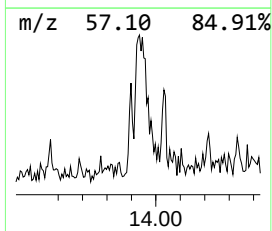
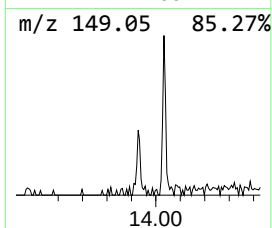
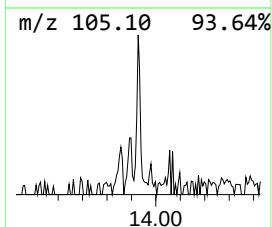
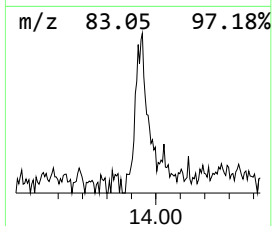
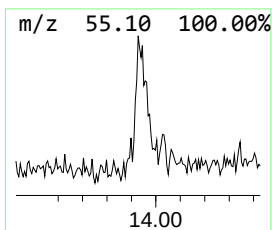
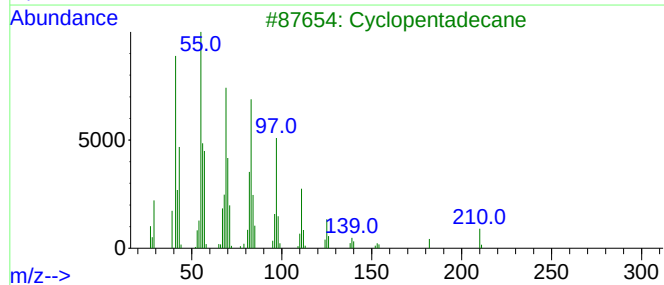
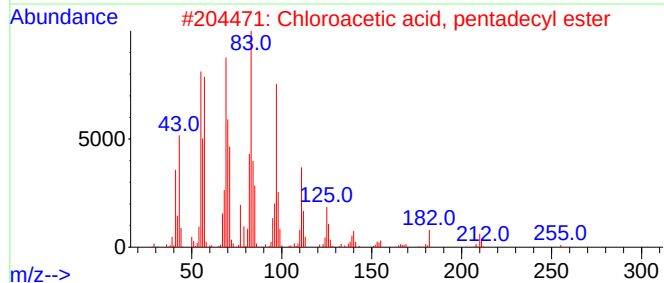
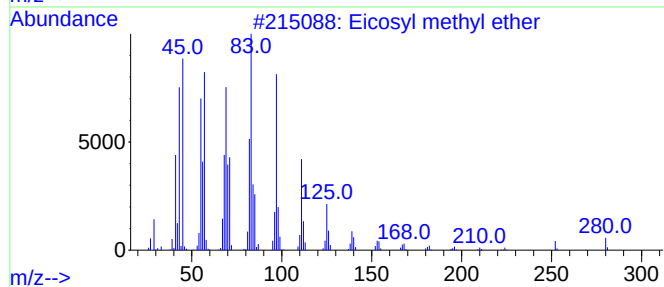
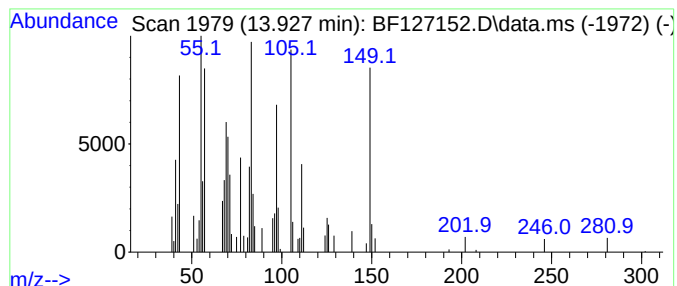
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Eicosyl methyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	4.46 ng	93452	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosyl methyl ether	312	C21H44O	1000406-29-4	64
2			Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	64
3			Cyclopentadecane	210	C15H30	000295-48-7	62
4			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	62
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	60



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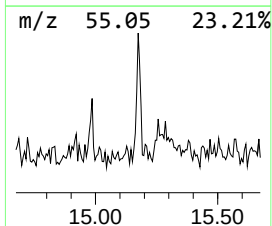
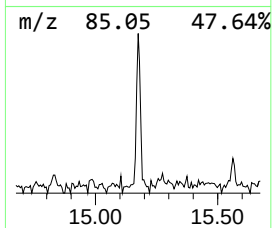
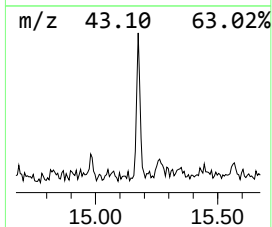
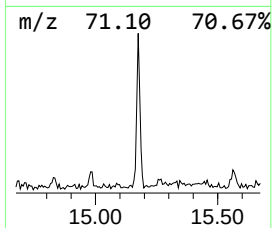
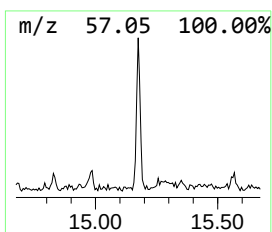
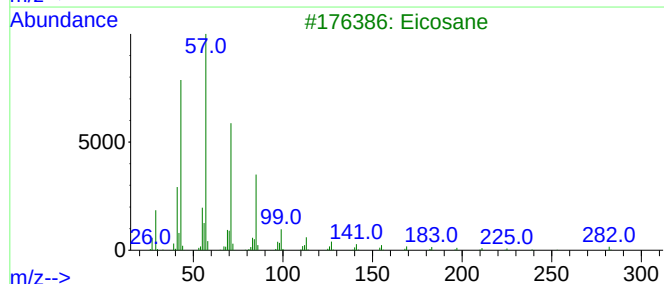
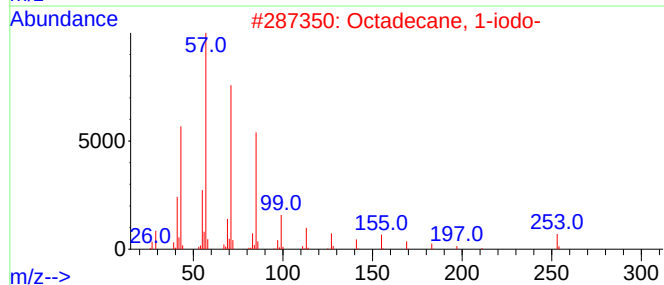
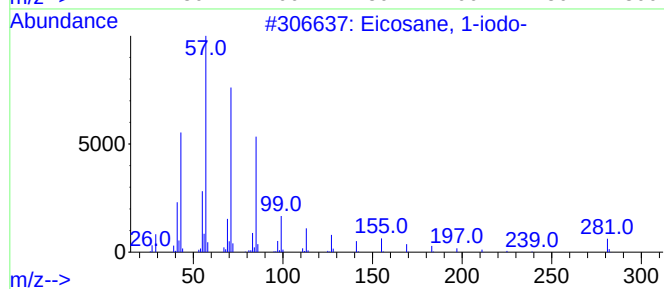
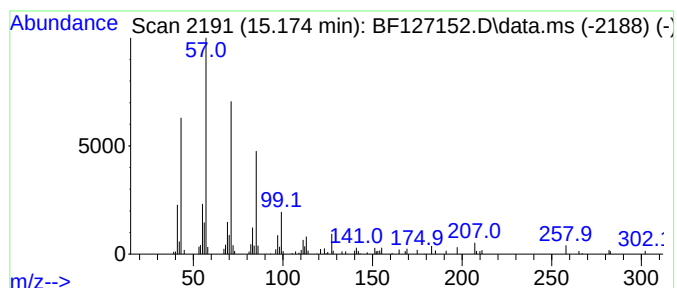
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Eicosane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	2.72 ng	66058	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
3			Eicosane	282	C20H42	000112-95-8	86
4			Heptadecane	240	C17H36	000629-78-7	80
5			Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	78



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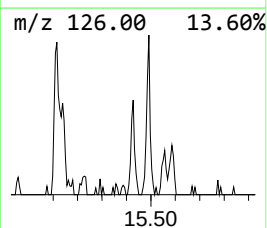
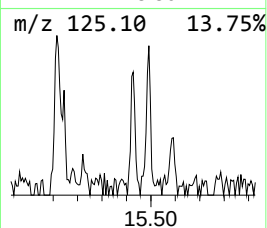
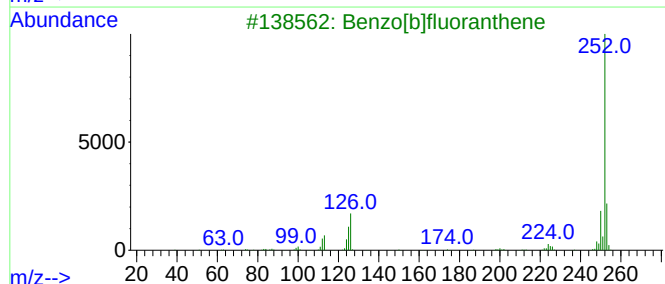
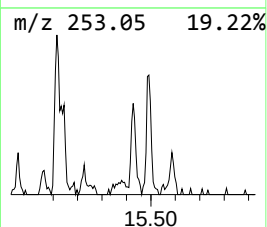
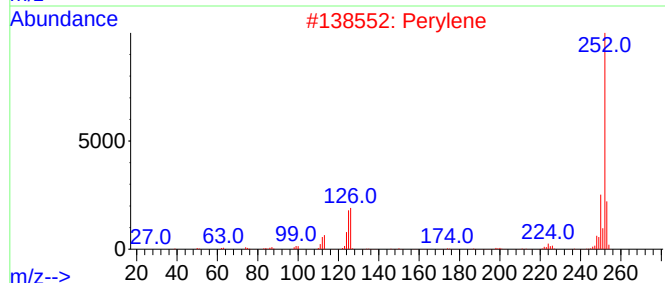
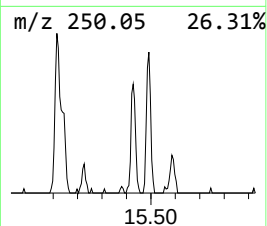
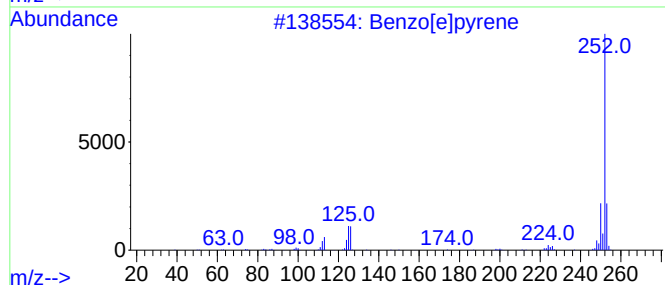
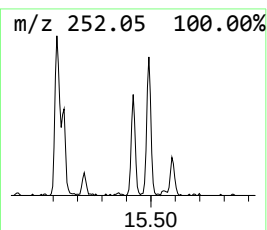
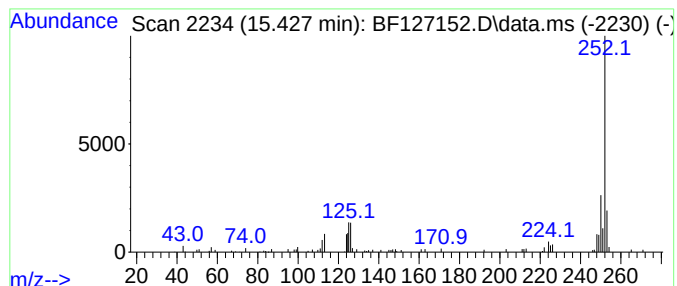
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	2.21 ng	53613	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	95
2			Perylene	252	C20H12	000198-55-0	95
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90



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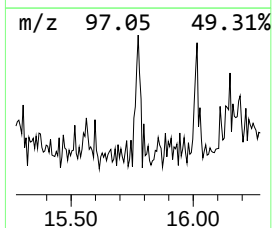
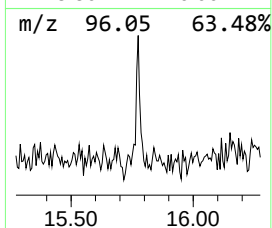
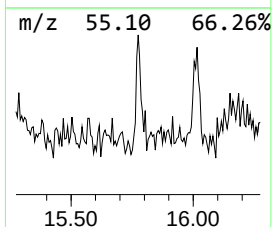
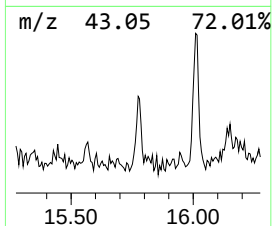
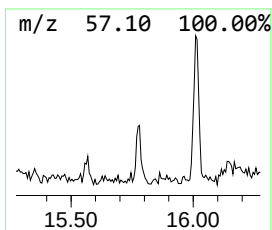
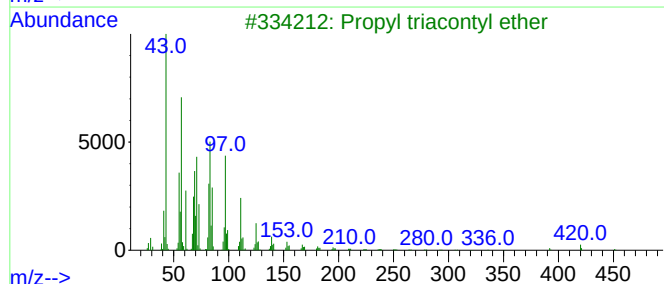
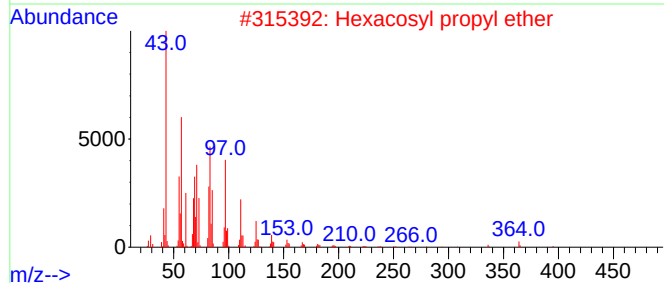
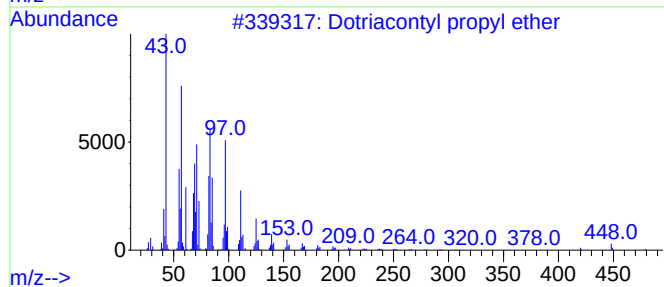
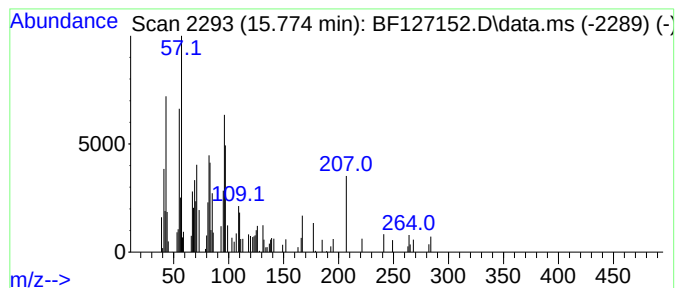
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.774 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	2.01 ng	48760	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontyl propyl ether	509	C35H72O	1000406-28-7	49
2			Hexacosyl propyl ether	424	C29H60O	1000406-28-4	46
3			Propyl triacontyl ether	481	C33H68O	1000406-28-6	46
4			Octacosyl propyl ether	452	C31H64O	1000406-28-5	46
5			Heptyl triacontyl ether	537	C37H76O	1000406-40-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030222\
Data File : BF127152.D
Acq On : 02 Mar 2022 17:39
Operator : CG\JU
Sample : N1721-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-4

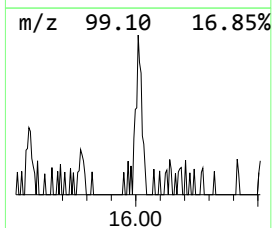
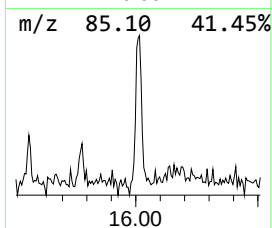
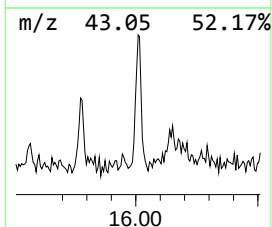
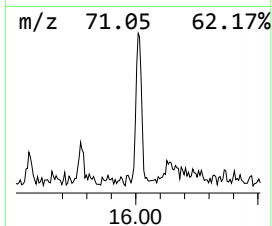
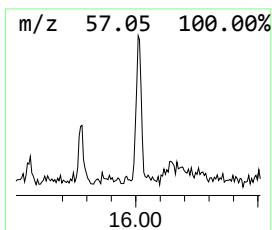
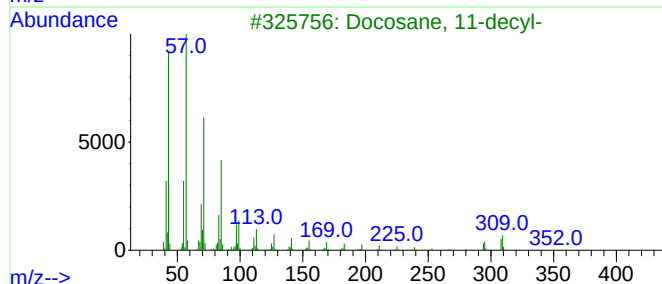
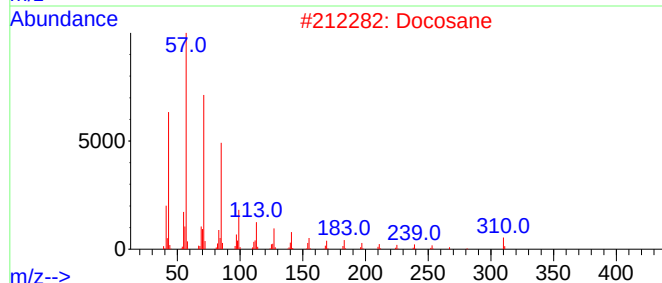
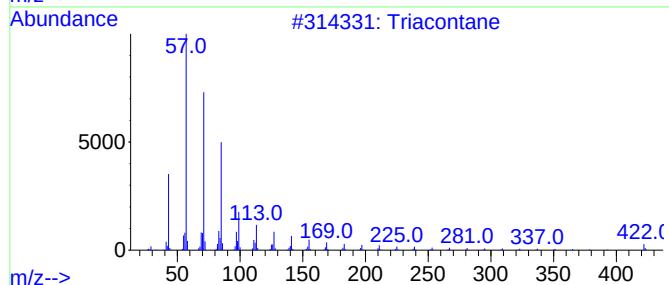
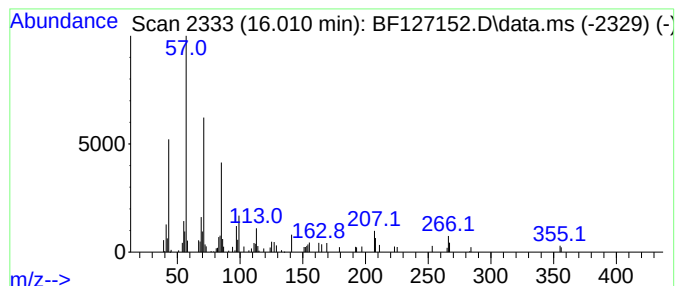
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	2.34 ng	56720	Perylene-d12	15.557

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	83
2		Docosane	310	C22H46	000629-97-0	83
3		Docosane, 11-decyl-	451	C32H66	055401-55-3	80
4		Octacosane	394	C28H58	000630-02-4	80
5		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030222\
Data File : BF127152.D
Acq On : 02 Mar 2022 17:39
Operator : CG\JU
Sample : N1721-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-4

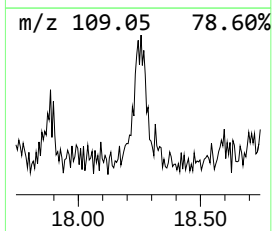
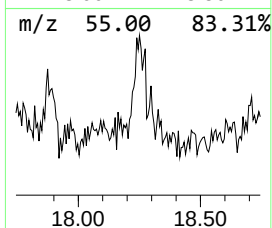
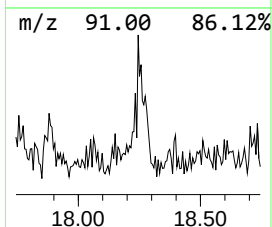
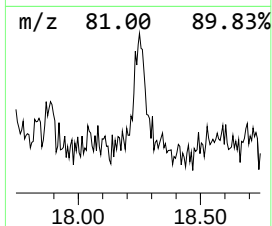
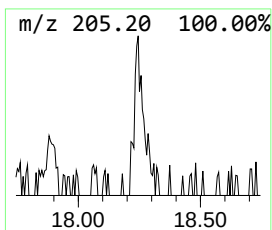
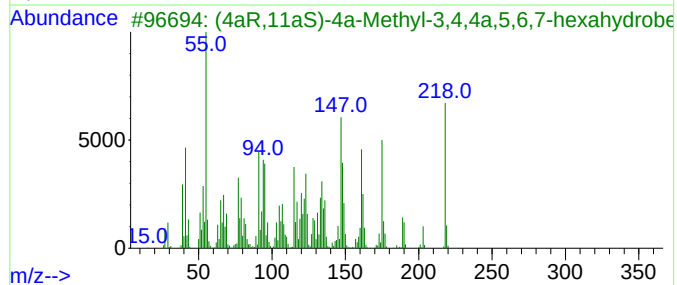
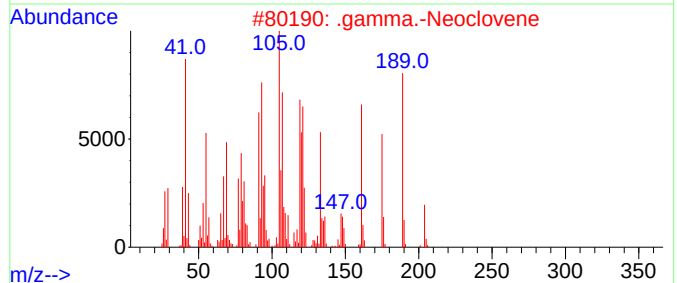
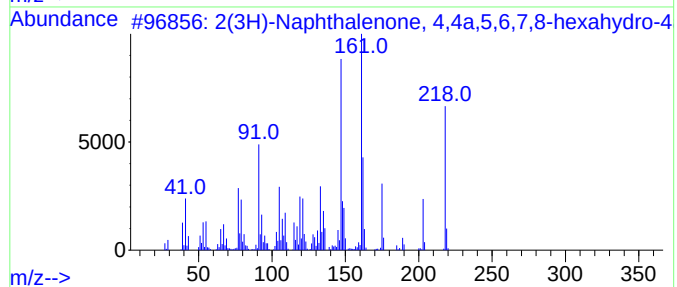
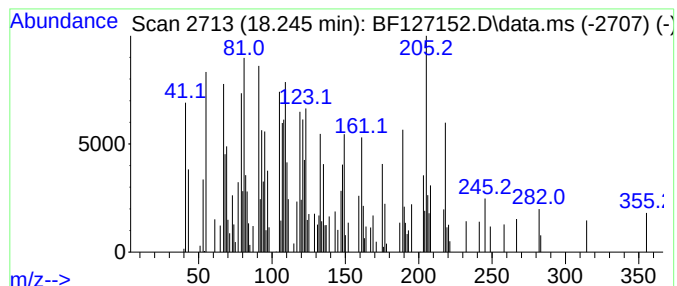
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.245 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.245	7.58 ng	184011	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Naphthalenone, 4,4a,5,6,7,...	218	C15H22O	019598-45-9	48		
2	.gamma.-Neoclovene	204	C15H24	1000156-11-7	45		
3	(4aR,11aS)-4a-Methyl-3,4,4a,5,6,...	218	C14H18O2	1000482-61-3	35		
4	(R)-2-((4aS,8aR)-4a-Methyl-8-met...	220	C15H24O	028102-68-3	25		
5	1H-Cyclopropa[a]naphthalene, dec...	204	C15H24	020071-49-2	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030222\
Data File : BF127152.D
Acq On : 02 Mar 2022 17:39
Operator : CG\JU
Sample : N1721-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
2-Pentanone, 4-...	5.116	5.2	ng	134442	1	6.887	513772	20.0
Ethanol, 2-(2-b...	8.069	2.5	ng	88750	2	8.169	696541	20.0
Eicosyl methyl ...	13.927	4.5	ng	93452	5	14.063	418959	20.0
Eicosane, 1-iodo-	15.174	2.7	ng	66058	6	15.557	485650	20.0
Benzo[e]pyrene	15.427	2.2	ng	53613	6	15.557	485650	20.0
unknown15.774	15.774	2.0	ng	48760	6	15.557	485650	20.0
Triacontane	16.010	2.3	ng	56720	6	15.557	485650	20.0
unknown18.245	18.245	7.6	ng	184011	6	15.557	485650	20.0