LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071421\
Data File : BP006231.D
Acq On : 14 Jul 2021 22:25
Operator : CG/JU
Sample : M3026-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : ABN-JG-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_P\Methods\8270E-BP070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006231.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.346	208	214	239	rVB	2878566	4281403	26.42%	5.607%
2	4.975	312	321	346	rBV	9278917	16208127	100.00%	21.225%
3	5.434	393	399	419	rBV	500266	930138	5.74%	1.218%
4	7.040	666	672	693	rBV	1211743	2403296	14.83%	3.147%
5	7.846	800	809	818	rBV	1001934	1659089	10.24%	2.173%
6	9.016	1001	1008	1031	rBV	1884511	3507639	21.64%	4.593%
7	10.452	1243	1252	1268	rBV2	144973	417197	2.57%	0.546%
8	10.646	1278	1285	1300	rBV	1302865	2366719	14.60%	3.099%
9	13.110	1696	1704	1720	rBV	5508652	8045785	49.64%	10.536%
10	14.487	1931	1938	1945	rBV	1872515	2915413	17.99%	3.818%
11	15.987	2188	2193	2204	rBV2	231829	439190	2.71%	0.575%
12	17.234	2399	2405	2409	rBV	2138529	3136878	19.35%	4.108%
13	17.275	2409	2412	2421	rVV	971803	1473109	9.09%	1.929%
14	17.375	2424	2429	2435	rVB	196082	310432	1.92%	0.407%
15	18.104	2549	2553	2558	rBV	123047	202263	1.25%	0.265%
16	18.151	2558	2561	2569	rVB	165468	226304	1.40%	0.296%
17	18.292	2580	2585	2589	rBV2	181921	316920	1.96%	0.415%
18	18.998	2699	2705	2709	rBV2	128669	239864	1.48%	0.314%
19	19.245	2741	2747	2752	rBV	1974656	2669061	16.47%	3.495%
20	19.563	2796	2801	2803	rBV3	435981	604827	3.73%	0.792%
21	19.592	2803	2806	2815	rVV	1802506	2399850	14.81%	3.143%
22	19.786	2833	2839	2845	rBV	7856148	9643515	59.50%	12.628%
23	19.910	2856	2860	2868	rVB2	91518	213739	1.32%	0.280%
24	20.075	2885	2888	2893	rVB	358434	432047	2.67%	0.566%
25	20.233	2909	2915	2918	rBV2	122240	228950	1.41%	0.300%
26	20.557	2967	2970	2976	rVB	258652	289221	1.78%	0.379%
27	20.969	3037	3040	3043	rBV2	152734	190502	1.18%	0.249%
28	21.010	3043	3047	3051	rVV2	731584	871241	5.38%	1.141%
29	21.310	3092	3098	3102	rBV2	2556189	4203307	25.93%	5.504%
30	21.351	3102	3105	3110	rVB	716020	889535	5.49%	1.165%
31	21.439	3117	3120	3123	rBV	194872	234239	1.45%	0.307%
32	22.969	3375	3380	3385	rBV	485562	1082977	6.68%	1.418%
33	23.586	3481	3485	3494	rVB	472880	890794	5.50%	1.167%
34	23.692	3497	3503	3509	rBV2	1227131	2440544	15.06%	3.196%

Sum of corrected areas: 76364115

Instrument :
BNA_P
ClientSampleId :
ABN-JG-2

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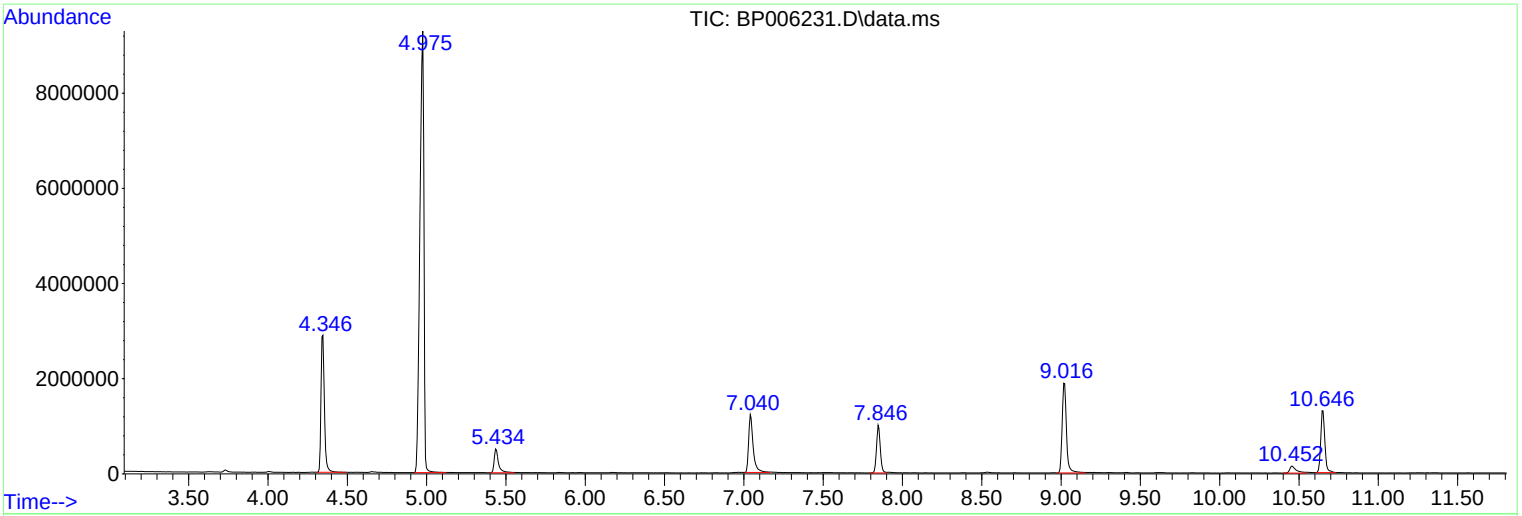
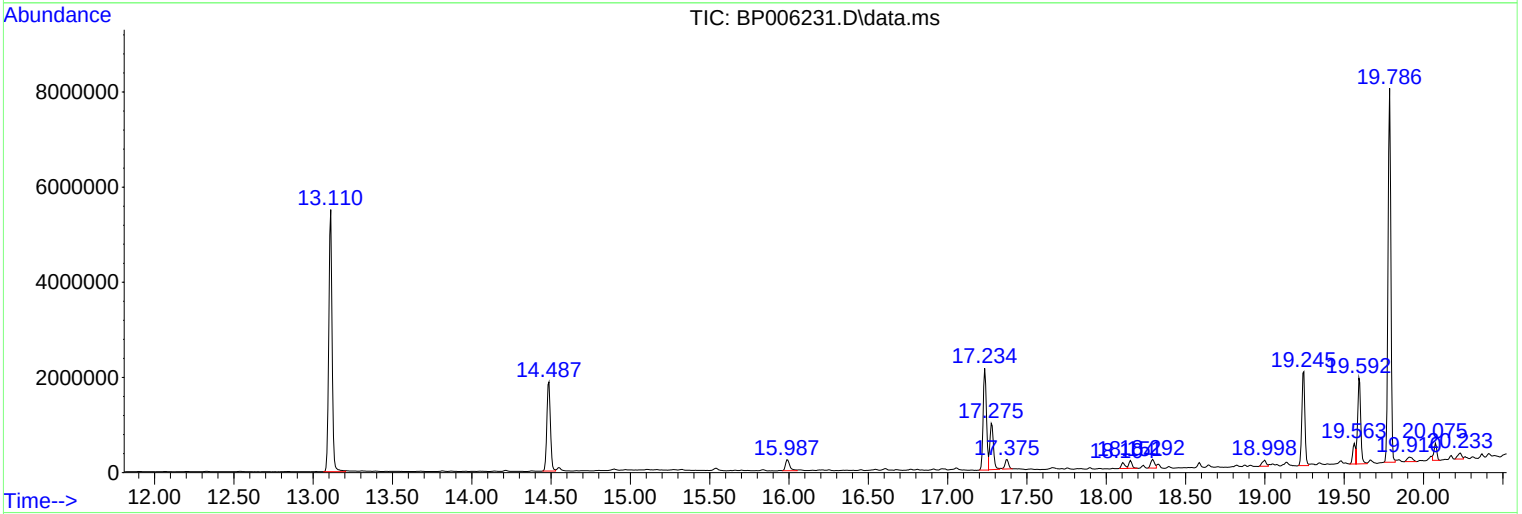
Misc :
ALS Vial : 18 Sample Multiplier: 1

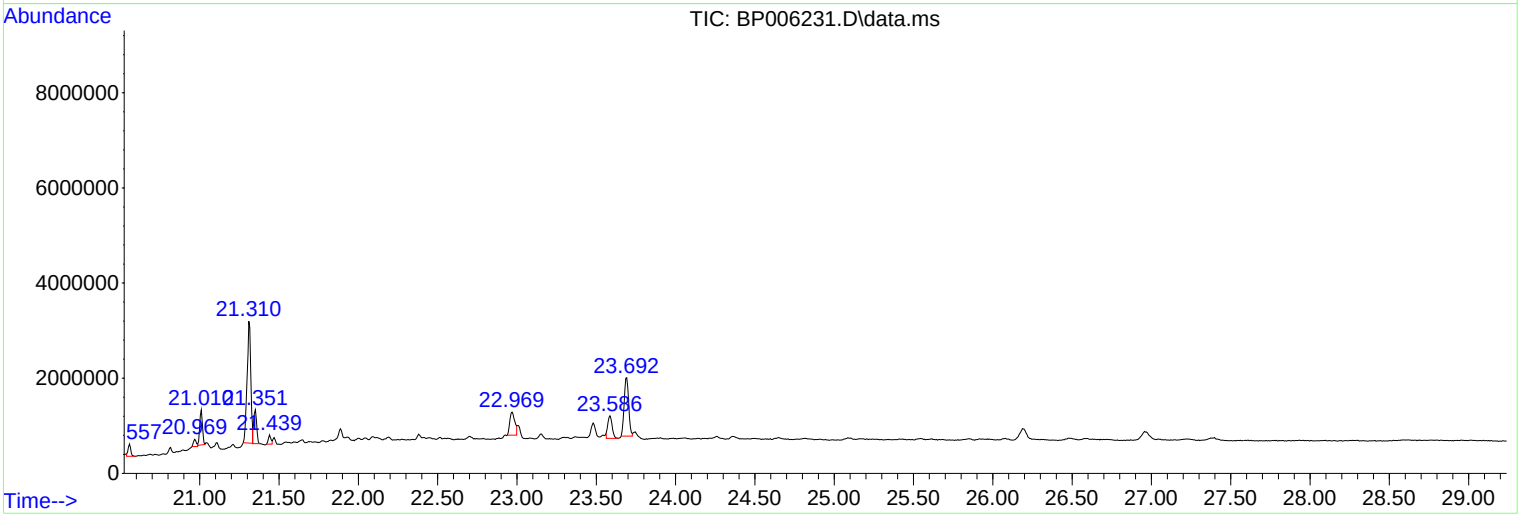
Instrument :
BNA_P
ClientSampleId :
ABN-JG-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.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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Data File : BP006231.D
Acq On : 14 Jul 2021 22:25
Operator : CG/JU
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Instrument : BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

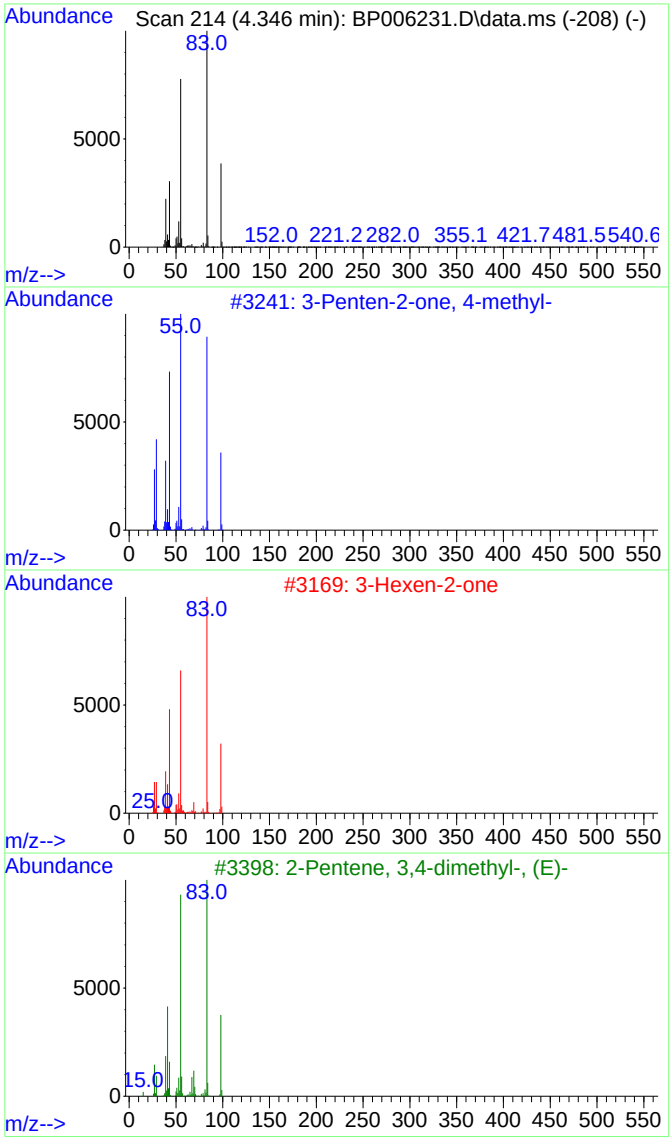
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

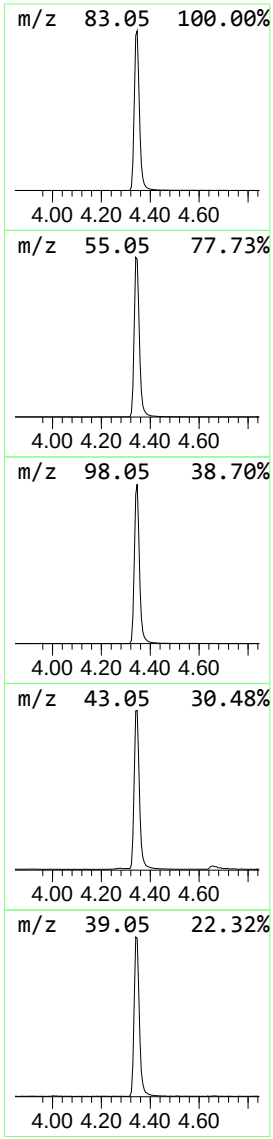
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.346	51.61 ng	4281400	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





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Operator : CG/JU
Sample : M3026-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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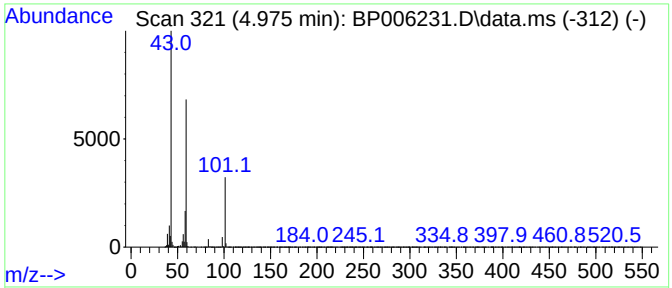
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

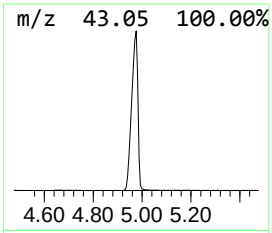
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

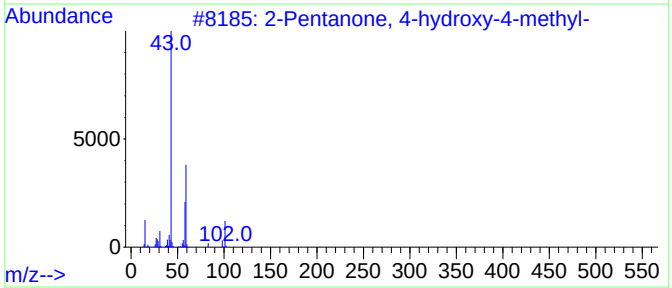
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

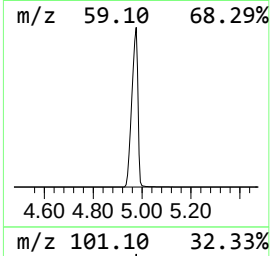
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	195.39 ng	16208100	1,4-Dichlorobenzene-d4	7.846

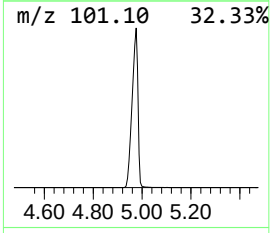
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Guanidine	59	CH5N3	000113-00-8	43
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17

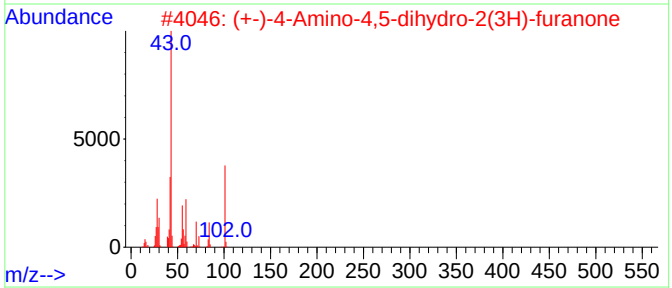


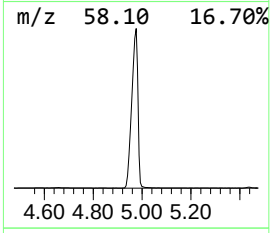


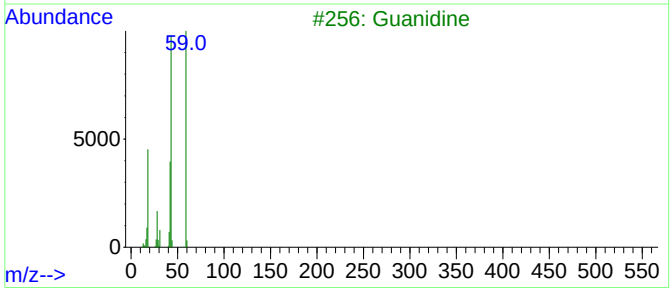


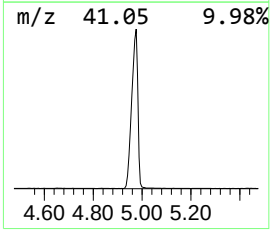












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Sample : M3026-05
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
ABN-JG-2

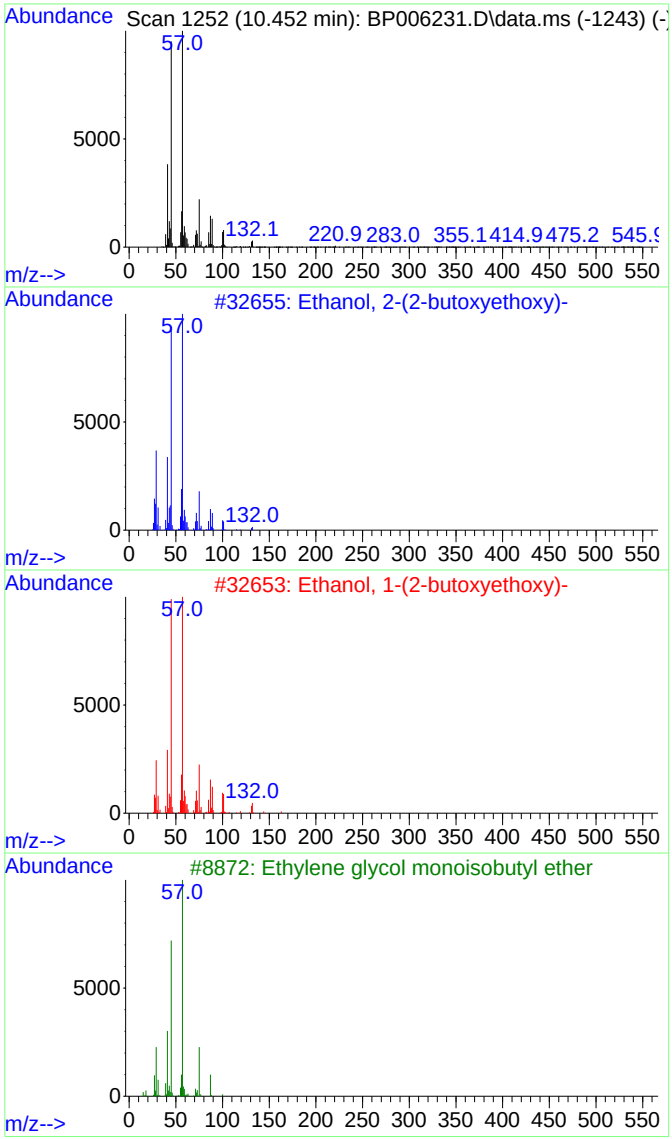
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

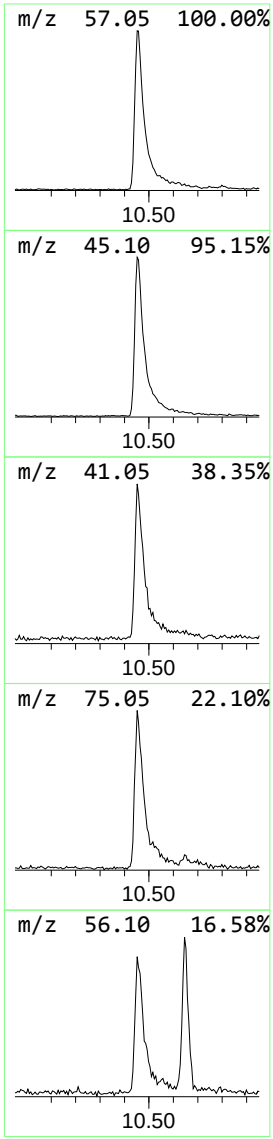
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.452	3.53 ng	417197	Naphthalene-d8	10.652

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	80
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52





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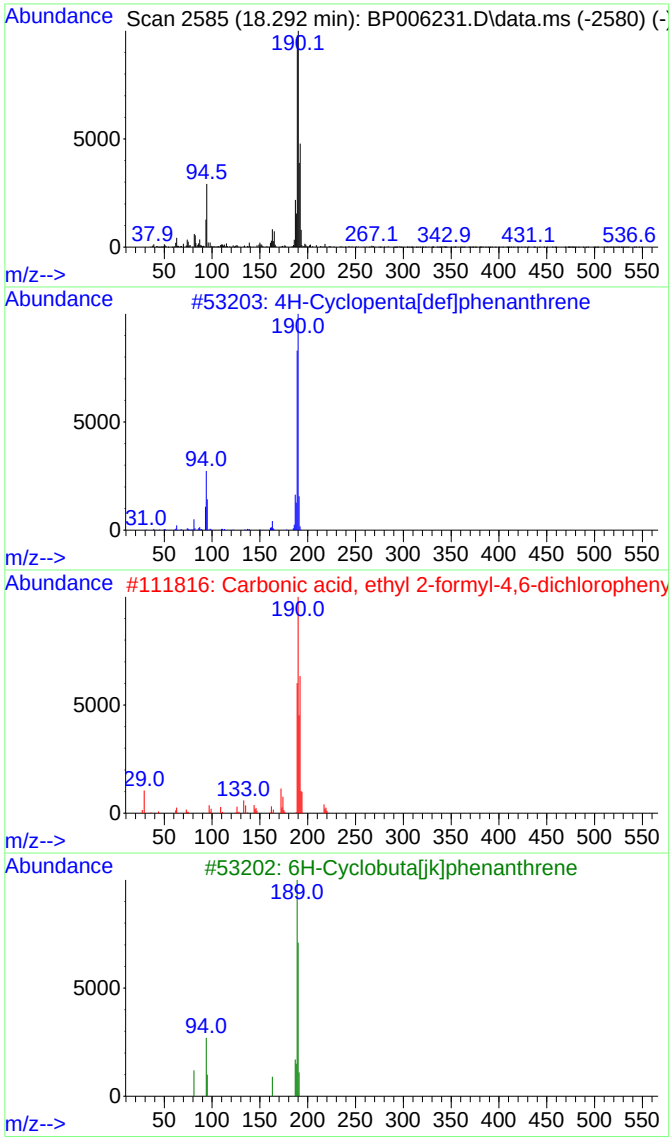
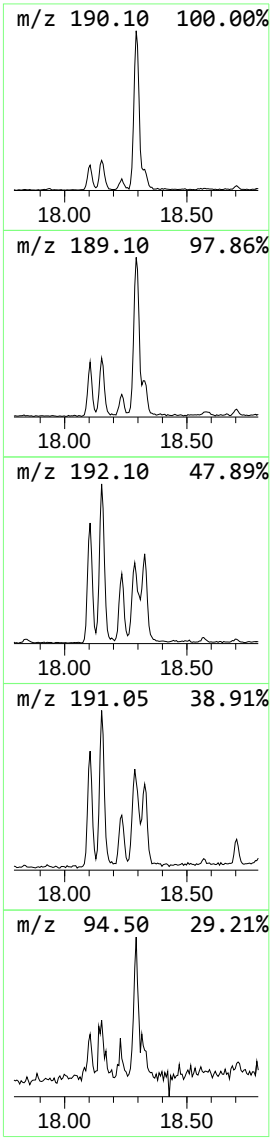
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.292	2.02 ng	316920	Phenanthrene-d10	17.234

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	42
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5	Methyl diselenide	190	C2H6Se2	007101-31-7	35





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ABN-JG-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

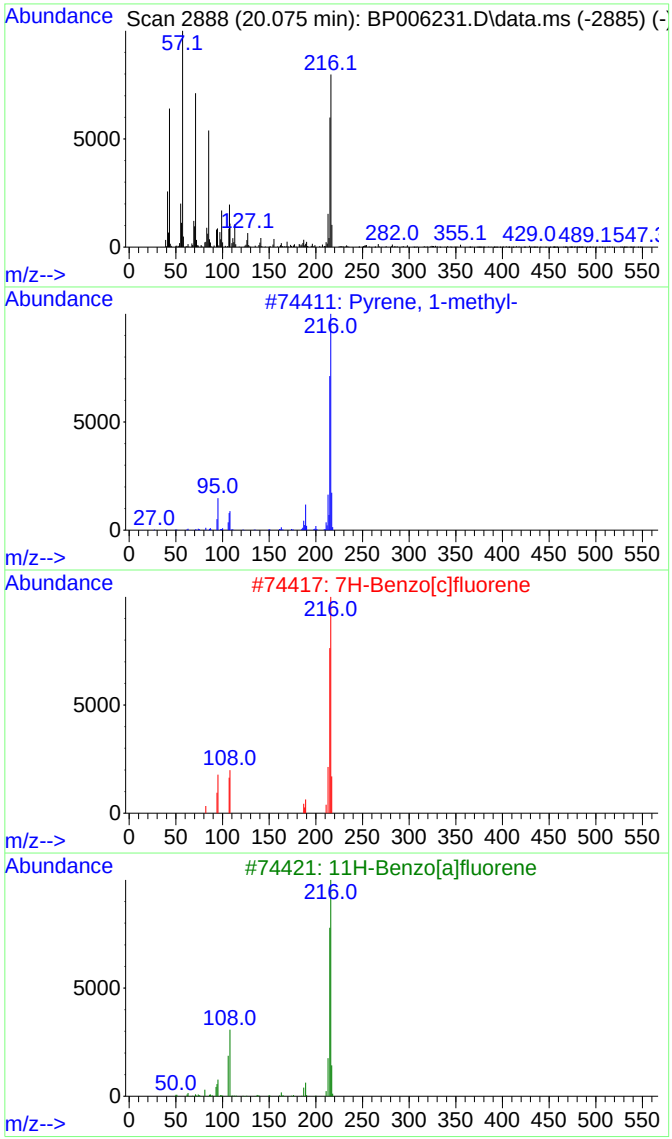
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

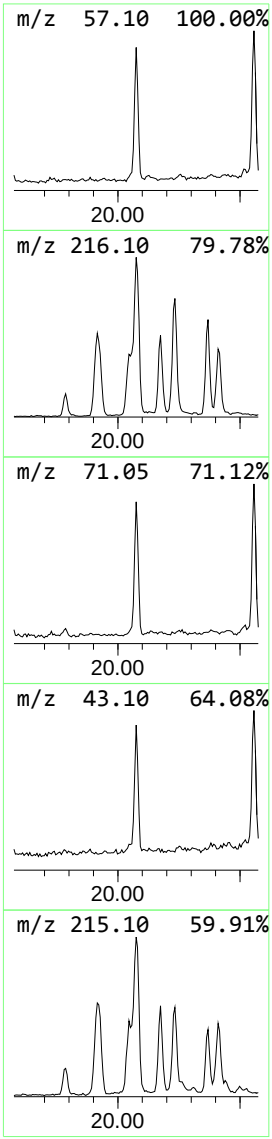
****

Peak Number 5 Pyrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.075	2.06 ng	432047	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	60
2	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	58
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	50
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	46
5	Pyrene, 4-methyl-	216	C17H12	003353-12-6	43





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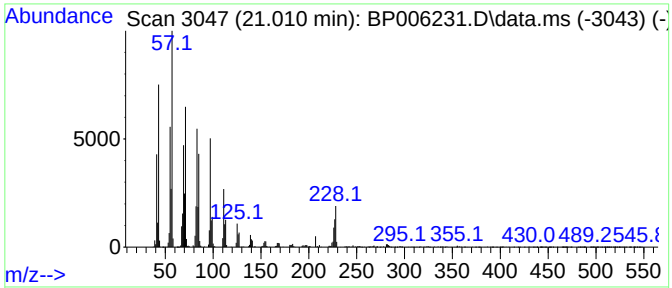
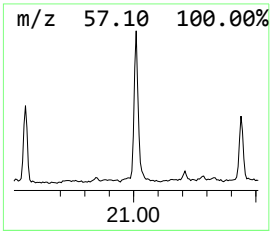
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

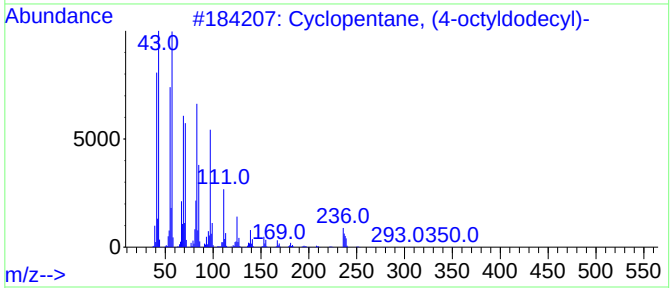
****
Peak Number 6 Cyclopentane, (4-octyldodec... Concentration Rank 3

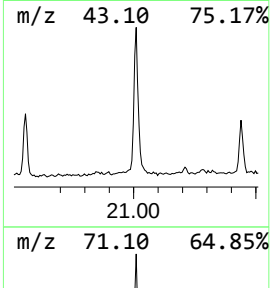
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	4.15 ng	871241	Chrysene-d12	21.316

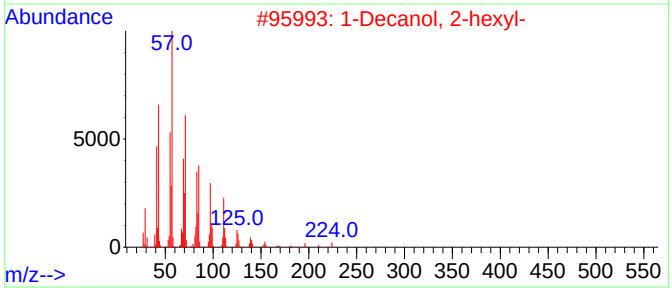
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	86
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	70
3	1-Octadecene	252	C18H36	000112-88-9	70
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	70
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	70

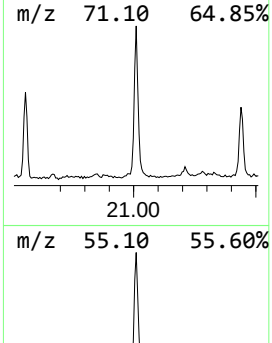


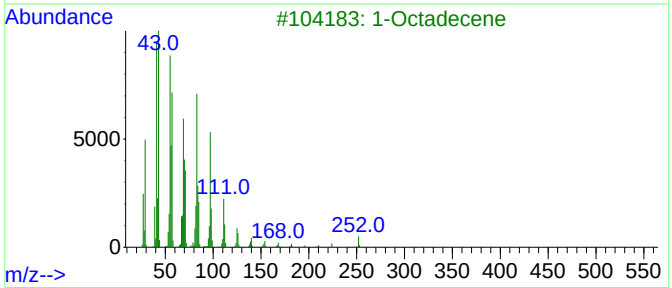


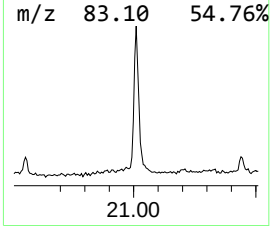












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071421\
Data File : BP006231.D
Acq On : 14 Jul 2021 22:25
Operator : CG/JU
Sample : M3026-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : ABN-JG-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one,...	4.346	51.6	ng	4281400	1	7.846	1659090	20.0
2-Pentanone, 4-...	4.975	195.4	ng	16208100	1	7.846	1659090	20.0
Ethanol, 2-(2-b...	10.452	3.5	ng	417197	2	10.652	2366720	20.0
4H-Cyclopenta[d...	18.292	2.0	ng	316920	4	17.234	3136880	20.0
Pyrene, 1-methyl-	20.075	2.1	ng	432047	5	21.316	4203310	20.0
Cyclopentane, (...	21.010	4.2	ng	871241	5	21.316	4203310	20.0