LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-02-040621

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-BP032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005230.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.287	369	374	380	rBV	63677	95151	30.23%	3.305%
2	5.716	443	447	452	rVB3	8954	12842	4.08%	0.446%
3	6.252	534	538	543	rBV4	4345	6631	2.11%	0.230%
4	6.328	548	551	555	rVV5	3037	4225	1.34%	0.147%
5	6.569	587	592	593	rBV3	3716	4367	1.39%	0.152%
6	6.687	608	612	616	rVB4	4805	7190	2.28%	0.250%
7	6.734	616	620	624	rBV4	4033	5365	1.70%	0.186%
8	6.781	624	628	631	rVV5	3236	4218	1.34%	0.146%
9	6.875	632	644	655	rVB	52641	108620	34.51%	3.772%
10	7.005	664	666	673	rVB6	2641	4718	1.50%	0.164%
11	7.069	673	677	681	rBV6	2707	4942	1.57%	0.172%
12	7.175	690	695	699	rBV3	3646	5994	1.90%	0.208%
13	7.240	703	706	710	rBV5	2538	3616	1.15%	0.126%
14	7.310	713	718	722	rBV	25740	39477	12.54%	1.371%
15	7.399	731	733	739	rVB7	2423	3158	1.00%	0.110%
16	7.693	774	783	790	rBV	83183	139713	44.39%	4.852%
17	7.805	798	802	805	rBV4	3122	3943	1.25%	0.137%
18	7.869	810	813	818	rVV5	4218	5966	1.90%	0.207%
19	7.963	822	829	838	rVB7	7110	17037	5.41%	0.592%
20	8.116	852	855	859	rBV5	2441	3309	1.05%	0.115%
21	8.216	864	872	873	rBV3	6162	10694	3.40%	0.371%
22	8.269	878	881	887	rVB3	5755	8140	2.59%	0.283%
23	8.346	887	894	905	rVB7	8581	21872	6.95%	0.760%
24	8.446	907	911	916	rBV3	6701	9201	2.92%	0.320%
25	8.510	918	922	927	rVB5	3400	4331	1.38%	0.150%
26	8.787	966	969	973	rVB6	6514	9213	2.93%	0.320%
27	8.852	973	980	985	rVV2	33437	59725	18.98%	2.074%
28	8.910	985	990	1000	rVB	36545	57457	18.25%	1.995%
29	8.999	1000	1005	1007	rBV5	3052	4595	1.46%	0.160%
30	9.040	1008	1012	1017	rVB6	4861	8794	2.79%	0.305%
31	9.375	1064	1069	1071	rBV5	3133	4893	1.55%	0.170%
32	9.604	1104	1108	1113	rVB4	3266	5209	1.65%	0.181%
33	9.651	1113	1116	1119	rBV4	2535	3563	1.13%	0.124%
34	9.828	1141	1146	1151	rVB7	2366	4128	1.31%	0.143%
35	9.904	1151	1159	1163	rBV10	3188	6505	2.07%	0.226%
36	10.481	1247	1257	1266	rBV	99368	176672	56.13%	6.136%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-02-040621

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-BP032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.963	1672	1679	1687	rBV	73595	114550	36.39%	3.978%
38	13.828	1819	1826	1831	rVB8	2427	5672	1.80%	0.197%
39	14.251	1894	1898	1903	rVB5	4391	6639	2.11%	0.231%
40	14.345	1908	1914	1924	rBV2	130804	205781	65.38%	7.147%
41	15.210	2053	2061	2067	rBV6	5192	8653	2.75%	0.301%
42	15.610	2125	2129	2134	rBV3	3814	5626	1.79%	0.195%
43	15.845	2163	2169	2179	rBV	49150	81283	25.82%	2.823%
44	16.075	2204	2208	2216	rBV4	8642	19069	6.06%	0.662%
45	16.469	2271	2275	2280	rVB7	2074	3645	1.16%	0.127%
46	16.875	2340	2344	2346	rBV3	6786	7812	2.48%	0.271%
47	16.922	2349	2352	2356	rVB4	4299	5859	1.86%	0.203%
48	17.110	2378	2384	2389	rBV	157428	235126	74.70%	8.166%
49	17.239	2403	2406	2411	rVB6	2502	3494	1.11%	0.121%
50	17.616	2465	2470	2474	rBV2	8216	11071	3.52%	0.384%
51	17.786	2495	2499	2505	rVB	41171	48428	15.39%	1.682%
52	18.004	2532	2536	2547	rVB6	13401	25123	7.98%	0.873%
53	18.169	2560	2564	2568	rBV6	2999	5185	1.65%	0.180%
54	18.292	2581	2585	2589	rBV3	7408	9594	3.05%	0.333%
55	18.369	2594	2598	2603	rBV7	2371	4158	1.32%	0.144%
56	18.686	2648	2652	2653	rBV4	2597	3456	1.10%	0.120%
57	18.898	2682	2688	2690	rBV	120802	154420	49.06%	5.363%
58	18.927	2690	2693	2697	rVB	128833	143664	45.64%	4.989%
59	19.057	2711	2715	2720	rVB2	25694	29941	9.51%	1.040%
60	19.127	2723	2727	2735	rVB	20288	31061	9.87%	1.079%
61	19.245	2741	2747	2751	rBV9	4705	10973	3.49%	0.381%
62	19.480	2782	2787	2796	rVB2	17891	34443	10.94%	1.196%
63	19.680	2816	2821	2826	rBV	136489	163720	52.02%	5.686%
64	20.122	2894	2896	2900	rBV5	5684	6623	2.10%	0.230%
65	20.921	3030	3032	3035	rBV4	11366	11594	3.68%	0.403%
66	21.210	3076	3081	3085	rBV	221179	292534	92.94%	10.159%
67	23.486	3462	3468	3476	rVB	160300	314755	100.00%	10.931%

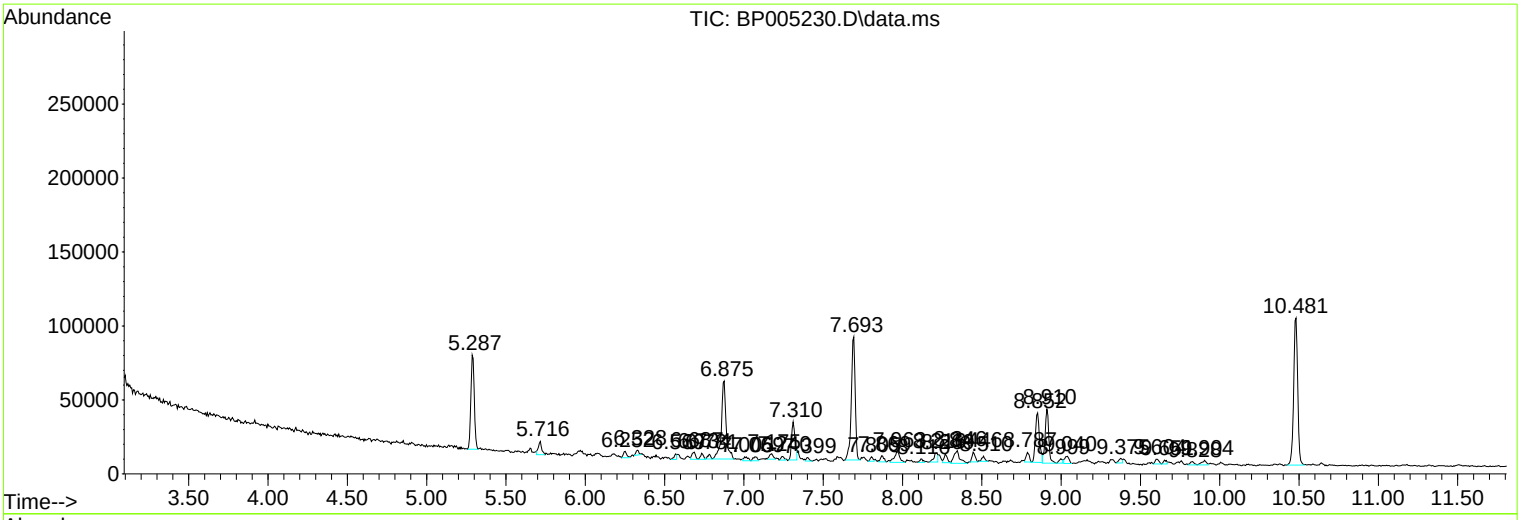
Sum of corrected areas: 2879426

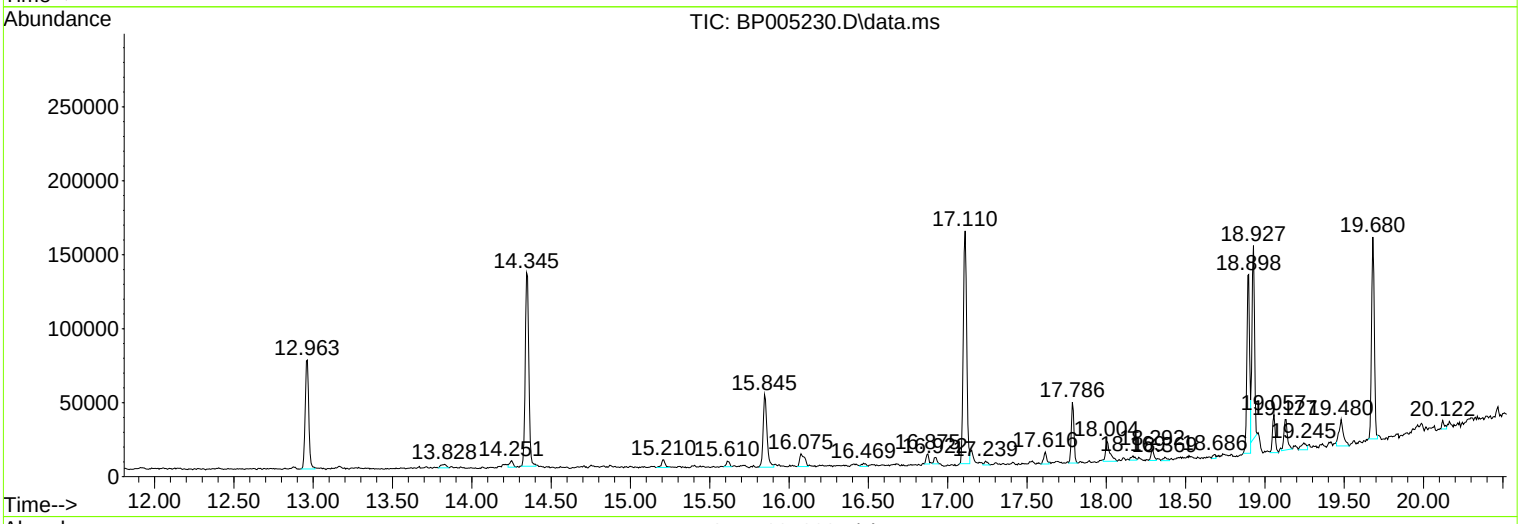
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

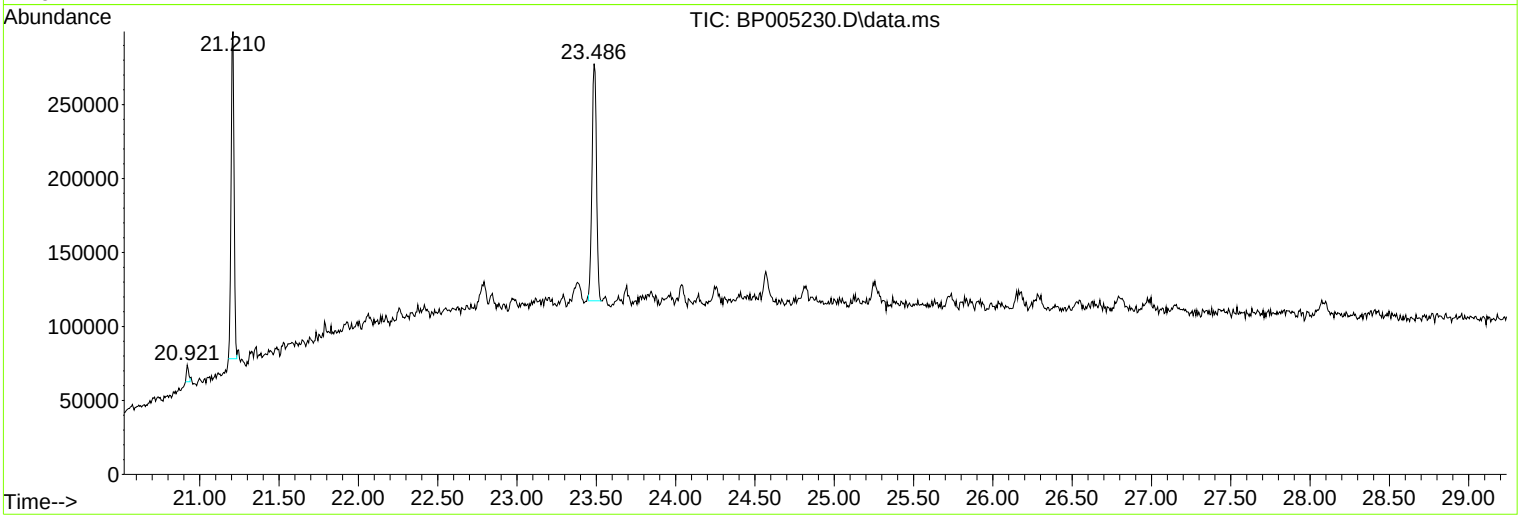
Instrument :
BNA_P
ClientSampleId :
HD-02-040621

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-02-040621

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

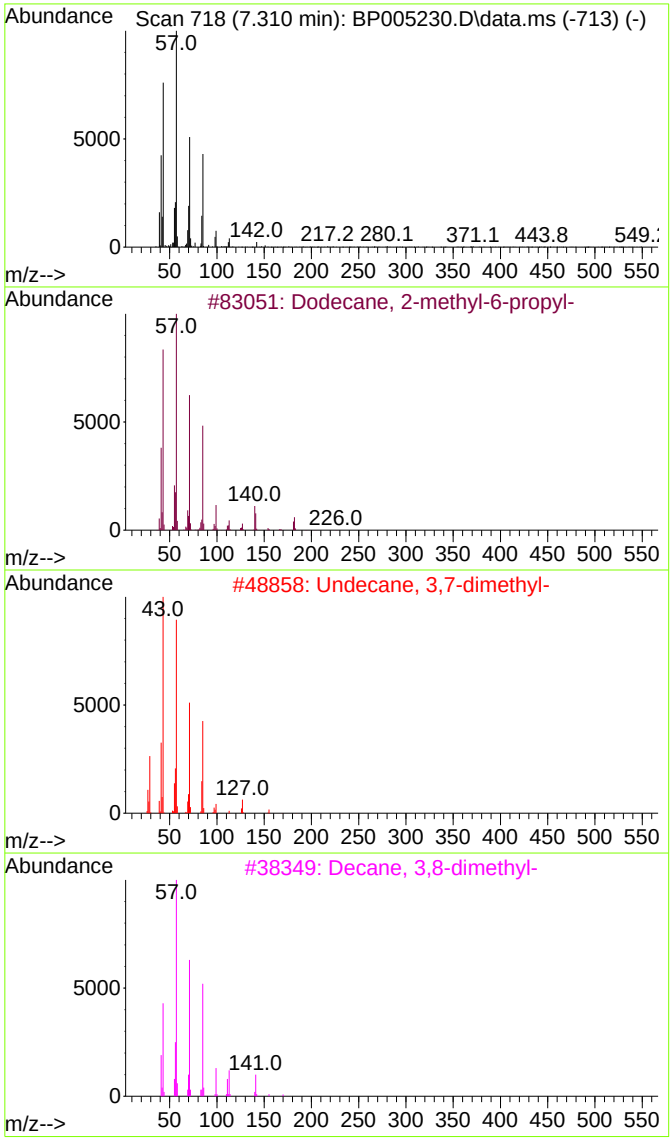
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

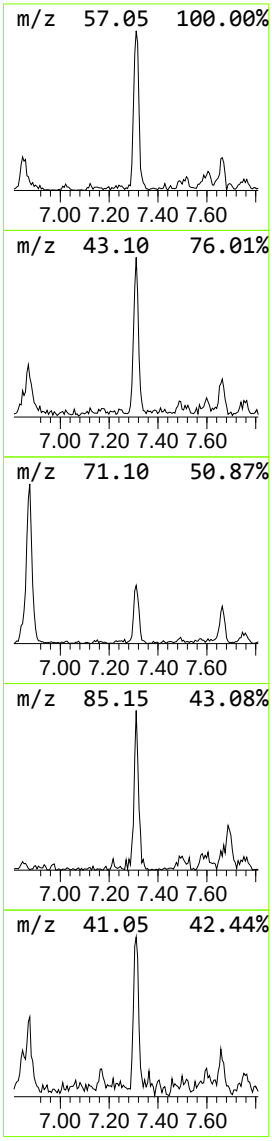
****

Peak Number 1 Dodecane, 2-methyl-6-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.310	5.65 ng	39477	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	74
2	Undecane, 3,7-dimethyl-	184	C13H28	017301-29-0	64
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
4	Tetradecane	198	C14H30	000629-59-4	64
5	Undecane, 4-ethyl-	184	C13H28	017312-59-3	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-02-040621

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

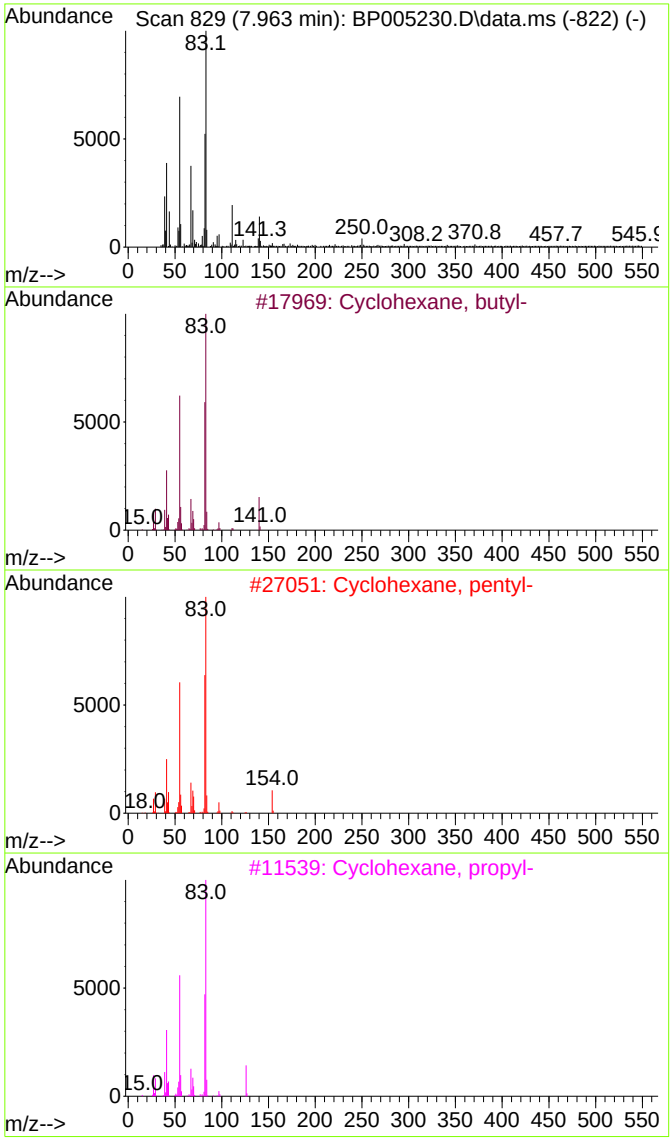
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

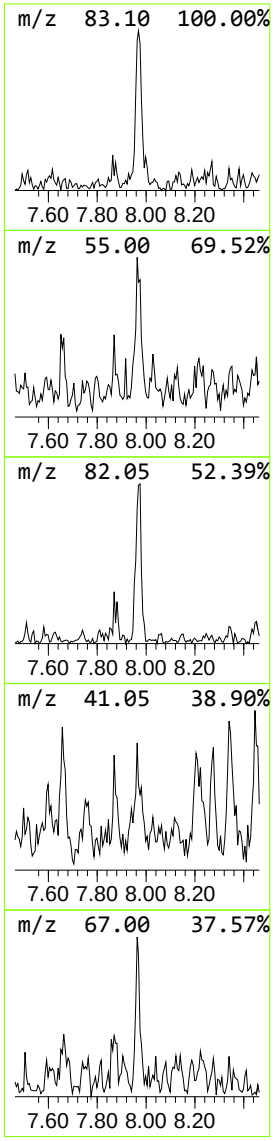
****

Peak Number 2 Cyclohexane, butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.963	2.44 ng	17037	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	76
2	Cyclohexane, pentyl-	154	C11H22	004292-92-6	64
3	Cyclohexane, propyl-	126	C9H18	001678-92-8	59
4	Cyclohexane, ethyl-	112	C8H16	001678-91-7	59
5	(1R,2R,4S)-2-(6-Chloropyridin-3-...	222	C12H15ClN2	232615-84-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-02-040621

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

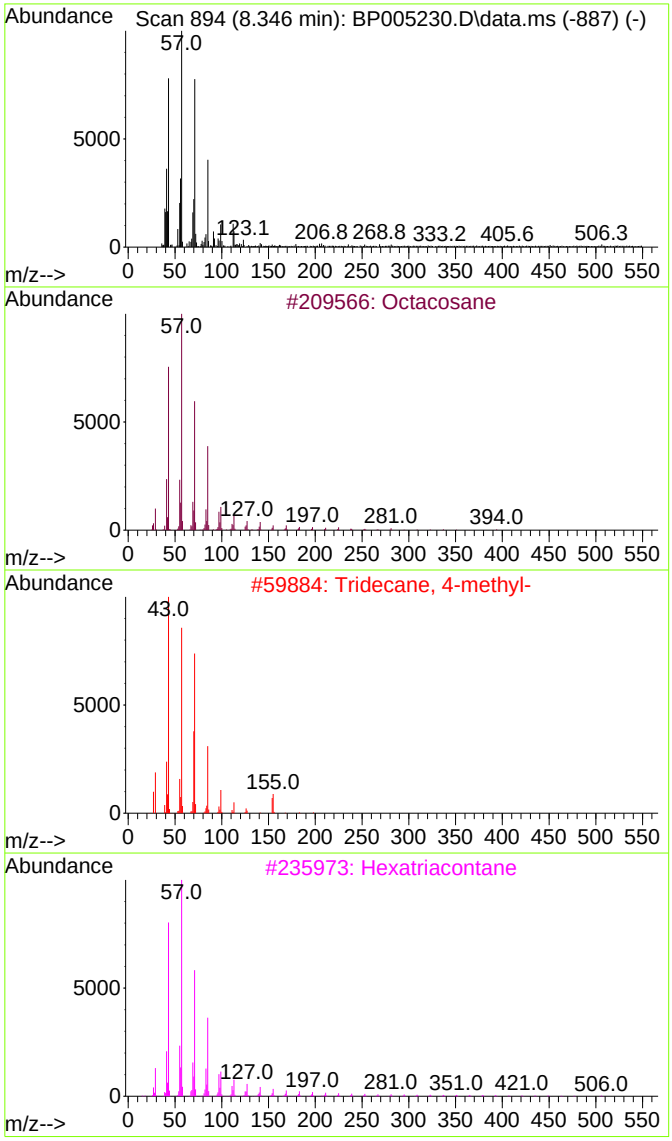
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

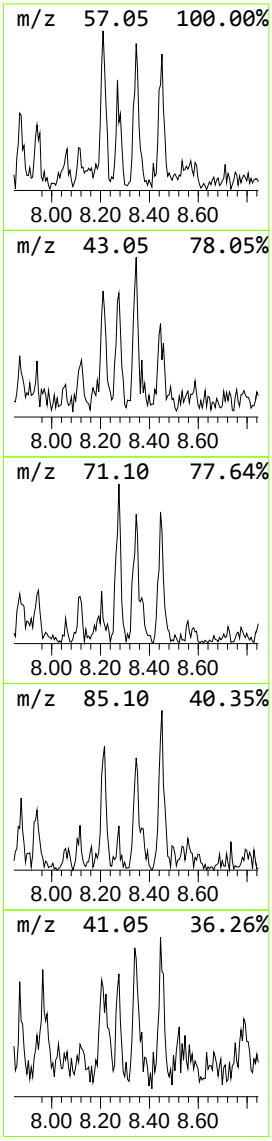
****

Peak Number 3 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.346	3.13 ng	21872	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	83
2	Tridecane, 4-methyl-	198	C14H30	026730-12-1	80
3	Hexatriacontane	507	C36H74	000630-06-8	80
4	Decane, 5-propyl-	184	C13H28	017312-62-8	80
5	Hexadecane	226	C16H34	000544-76-3	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-02-040621

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

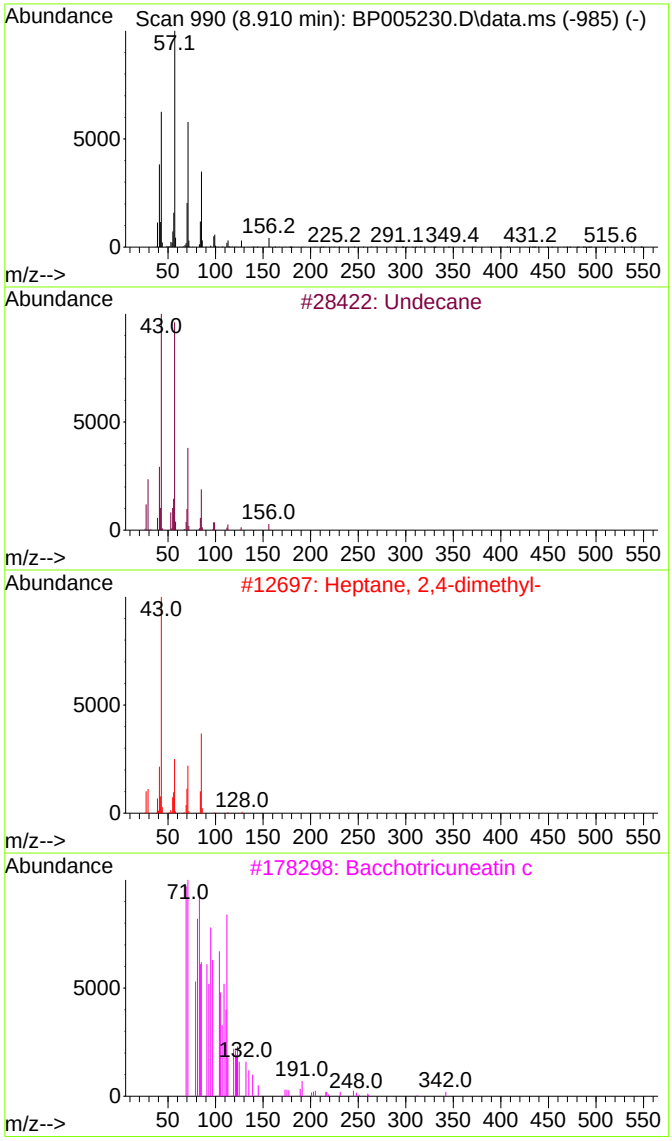
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

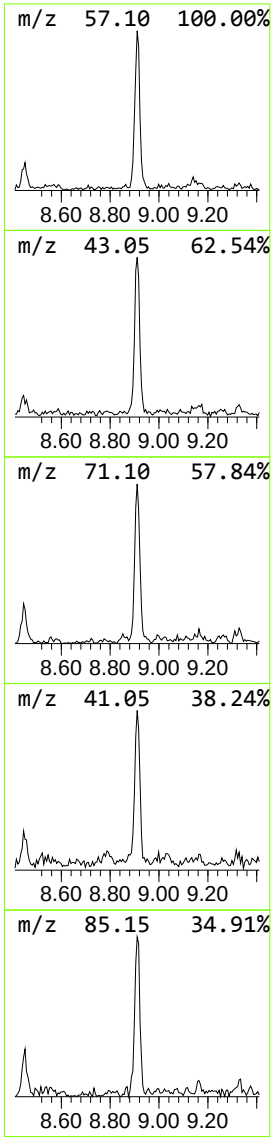
****

Peak Number 4 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.910	8.22 ng	57457	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	87
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64
4	Tridecane	184	C13H28	000629-50-5	64
5	1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-02-040621

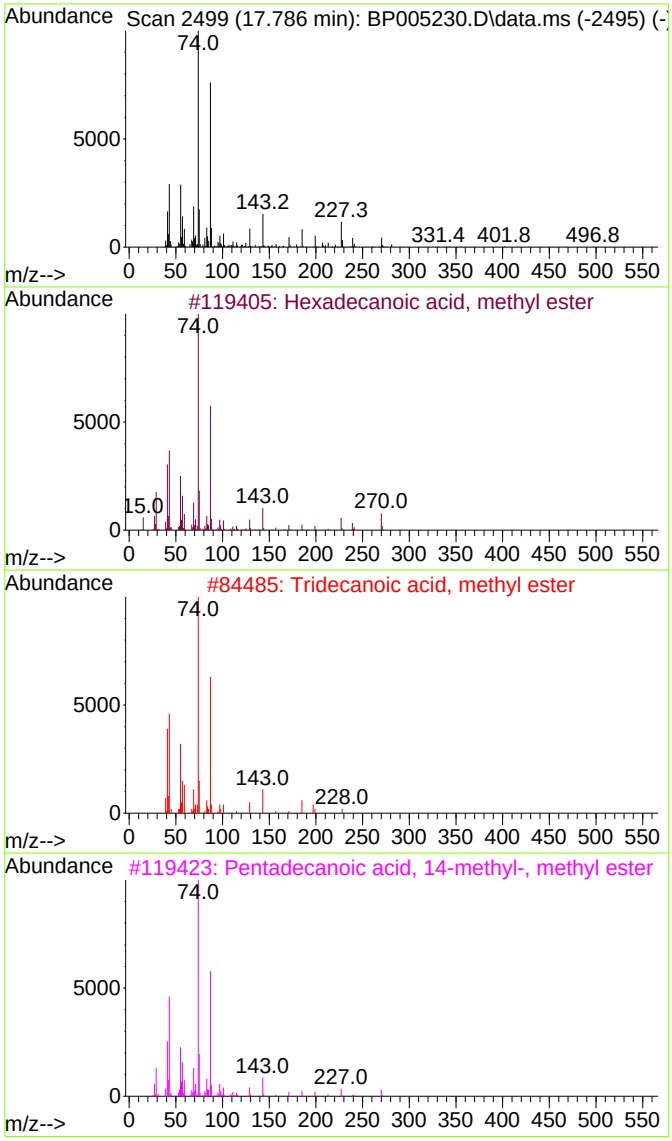
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

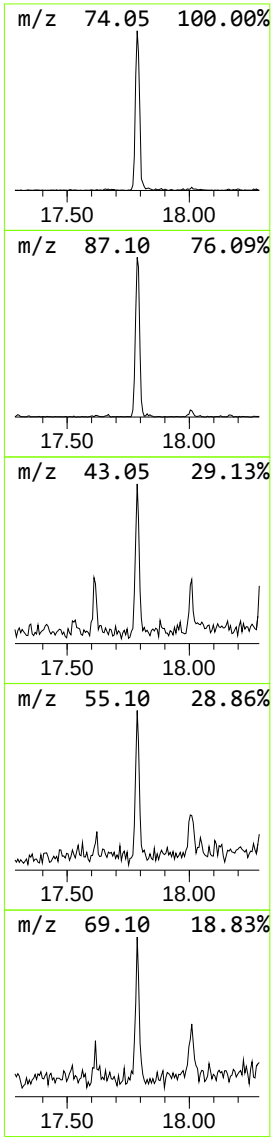
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.786	4.12 ng	48428	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-02-040621

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

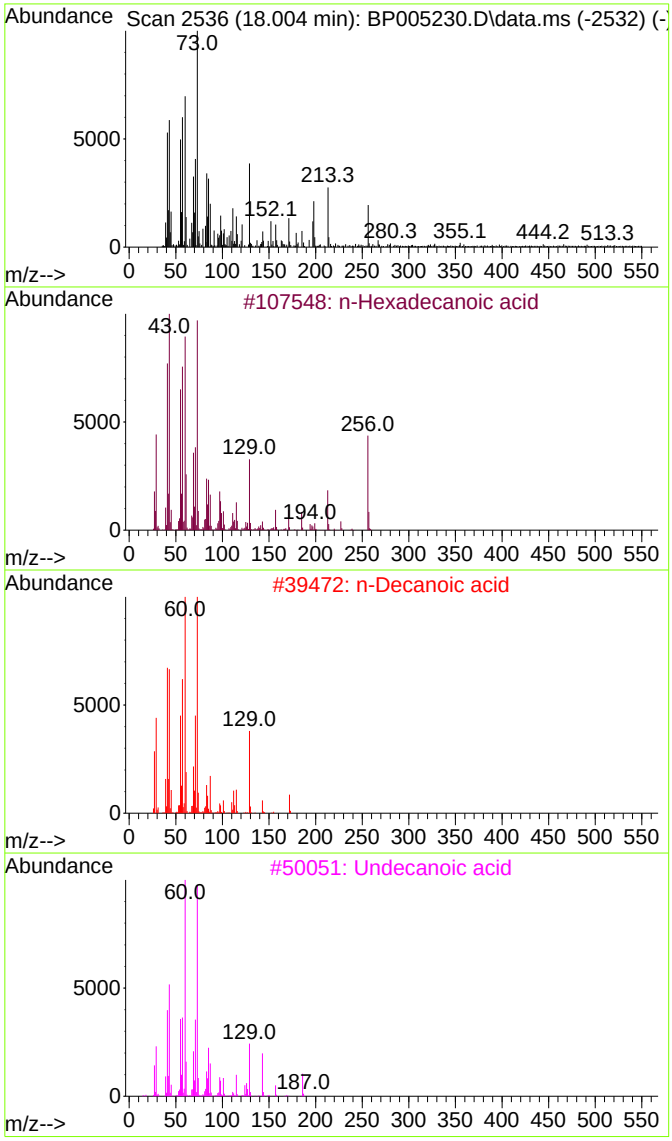
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

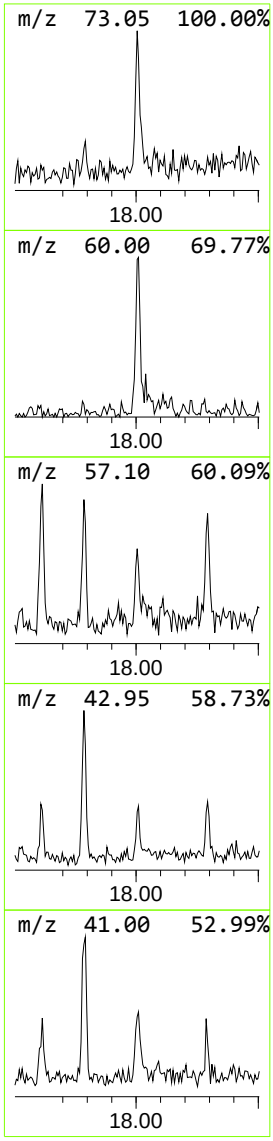
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.004	2.14 ng	25123	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-02-040621

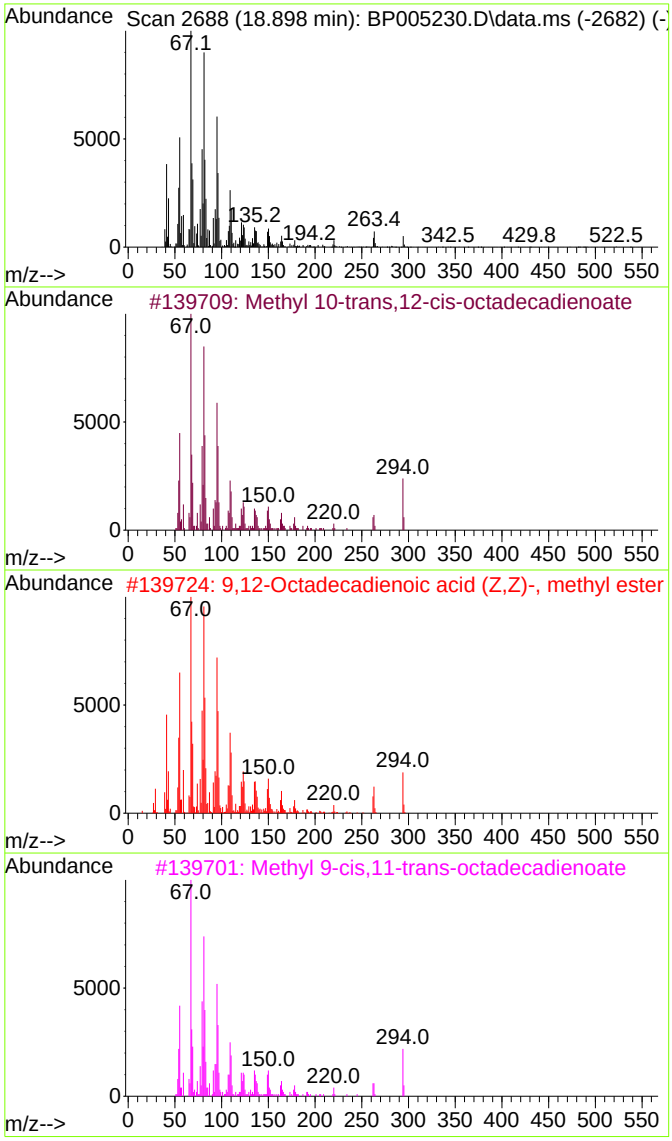
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

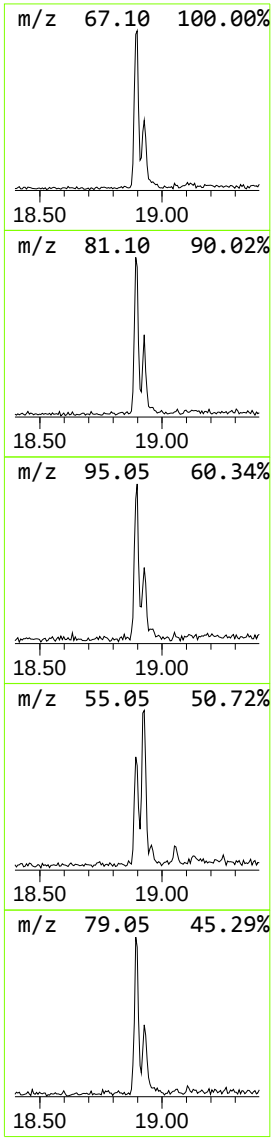
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Methyl 10-trans,12-cis-octa... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.898	13.14 ng	154420	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	97
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	96





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Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-02-040621

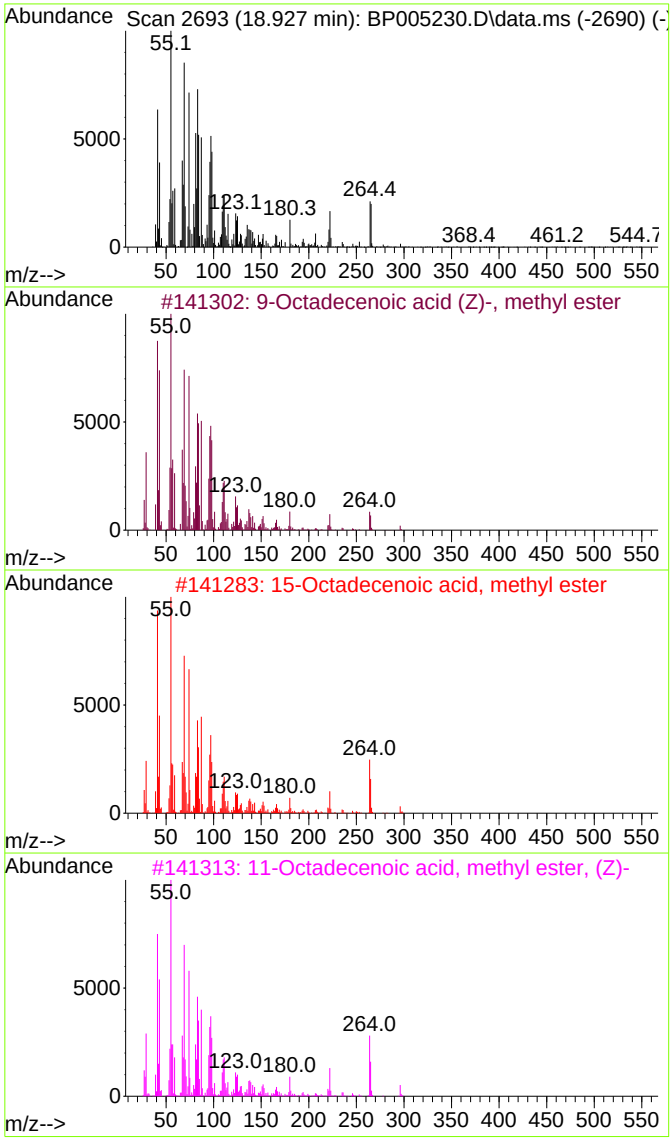
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

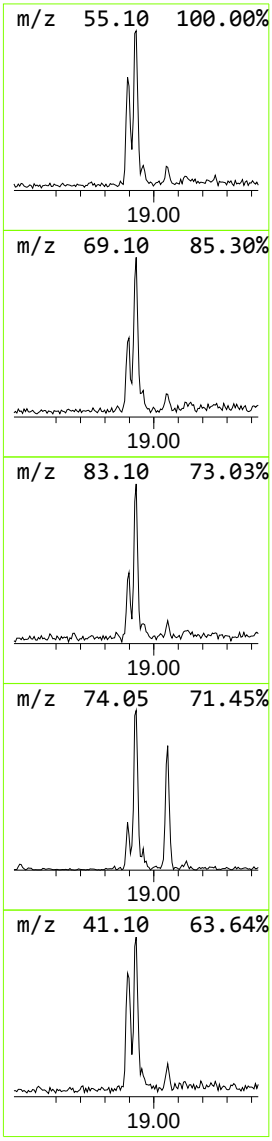
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.927	12.22 ng	143664	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	95
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	95
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	95
5	n-Propyl 9-octadecenoate	324	C21H40O2	1000336-71-6	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-02-040621

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

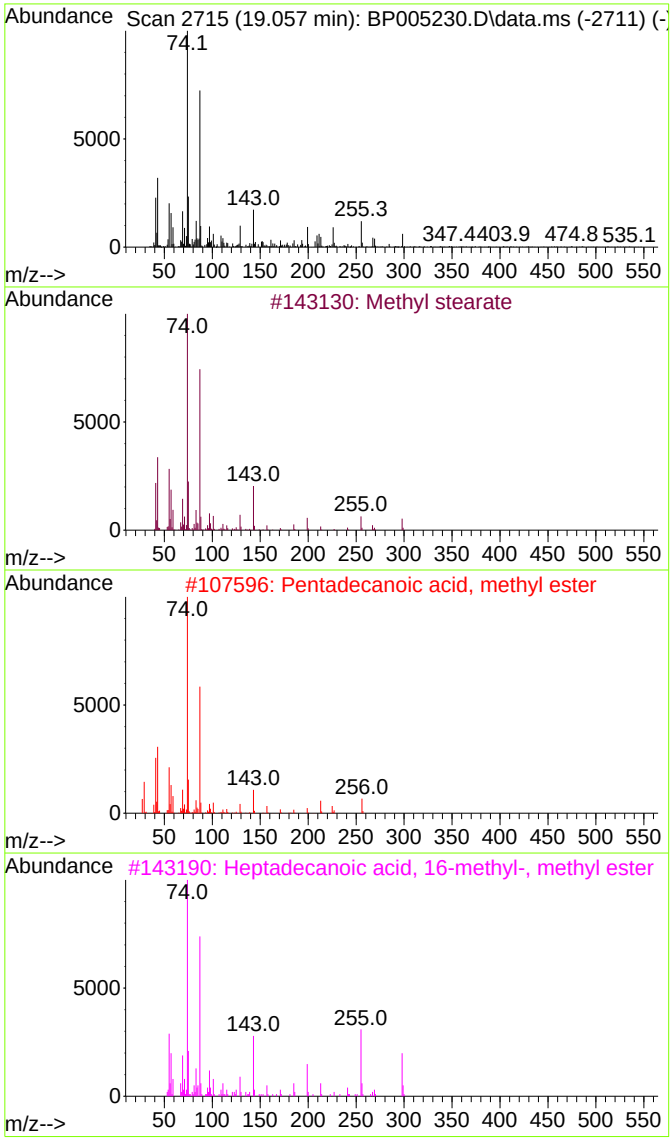
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

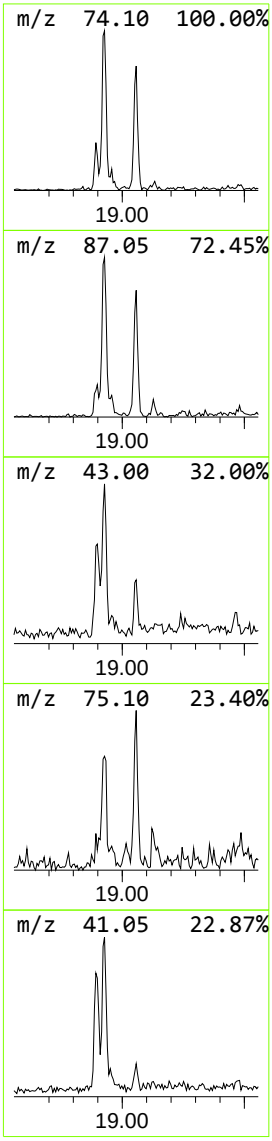
****

Peak Number 9 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.057	2.55 ng	29941	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	93
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-02-040621

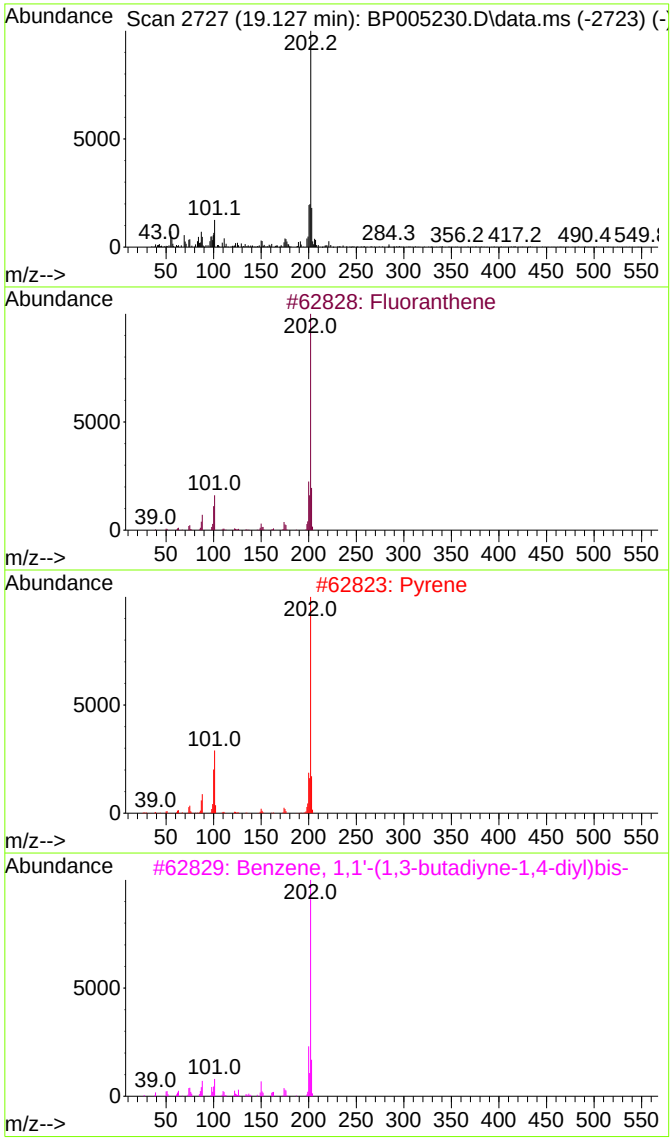
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

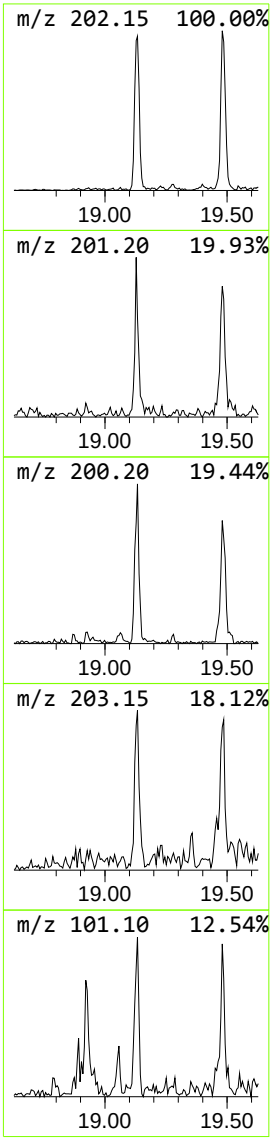
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.127	2.64 ng	31061	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	89
2	Pyrene	202	C16H10	000129-00-0	74
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	58
4	1-Methyl-7,11-dithiaspiro[5,5] u...	202	C10H18S2	107678-22-8	46
5	4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005230.D
Acq On : 07 Apr 2021 20:33
Operator : CG/JU
Sample : M1953-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-02-040621

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.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
Dodecane, 2-met...	7.310	5.7	ng	39477	1	7.693	139713	20.0
Cyclohexane, bu...	7.963	2.4	ng	17037	1	7.693	139713	20.0
Octacosane	8.346	3.1	ng	21872	1	7.693	139713	20.0
Undecane	8.910	8.2	ng	57457	1	7.693	139713	20.0
Hexadecanoic ac...	17.786	4.1	ng	48428	4	17.110	235126	20.0
n-Hexadecanoic ...	18.004	2.1	ng	25123	4	17.110	235126	20.0
Methyl 10-trans...	18.898	13.1	ng	154420	4	17.110	235126	20.0
9-Octadecenoic ...	18.927	12.2	ng	143664	4	17.110	235126	20.0
Methyl stearate	19.057	2.5	ng	29941	4	17.110	235126	20.0
Benzene, 1,1'-(...	19.127	2.6	ng	31061	4	17.110	235126	20.0