LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

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_E\Methods\8270-BE110624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BE101519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.672	11	14	27	rVB	334267	388975	13.05%	1.334%
2	2.866	43	47	55	rBV	140045	166127	5.57%	0.570%
3	4.787	371	374	386	rBV	18174	35700	1.20%	0.122%
4	5.310	456	463	485	rBV	449475	776164	26.03%	2.661%
5	6.937	732	740	760	rBV	432534	840466	28.19%	2.882%
6	7.072	760	763	776	rVB2	15837	32142	1.08%	0.110%
7	7.560	839	846	854	rBV	263619	434994	14.59%	1.491%
8	8.765	1044	1051	1071	rBV	300395	535584	17.96%	1.836%
9	9.716	1205	1213	1219	rBV3	20403	39493	1.32%	0.135%
10	10.322	1309	1316	1323	rBV	402199	718745	24.11%	2.464%
11	11.967	1590	1596	1604	rBV	26014	46350	1.55%	0.159%
12	12.196	1629	1635	1653	rVB3	16195	42033	1.41%	0.144%
13	12.789	1729	1736	1744	rBV	1040132	1529400	51.30%	5.244%
14	13.318	1817	1826	1833	rBV4	13329	38571	1.29%	0.132%
15	13.471	1846	1852	1856	rBV	17447	31904	1.07%	0.109%
16	13.518	1856	1860	1870	rVB2	17814	33359	1.12%	0.114%
17	13.900	1917	1925	1940	rBV	53901	125012	4.19%	0.429%
18	14.164	1964	1970	1977	rVB	735292	1089359	36.54%	3.735%
19	14.752	2061	2070	2075	rBV3	15989	37112	1.24%	0.127%
20	15.210	2145	2148	2158	rBV3	15916	32077	1.08%	0.110%
21	15.533	2199	2203	2215	rVB	66557	102508	3.44%	0.351%
22	15.674	2216	2227	2234	rBV	1002729	1473136	49.41%	5.051%
23	15.733	2234	2237	2245	rVB2	18108	32822	1.10%	0.113%
24	15.933	2265	2271	2278	rBV6	14598	33303	1.12%	0.114%
25	16.579	2373	2381	2385	rBV	25672	55402	1.86%	0.190%
26	16.720	2401	2405	2410	rBV	27822	45038	1.51%	0.154%
27	16.808	2416	2420	2428	rBV2	44733	94466	3.17%	0.324%
28	16.902	2428	2436	2440	rVV	956092	1450632	48.65%	4.974%
29	16.943	2440	2443	2448	rVB	401040	521909	17.50%	1.789%
30	17.031	2453	2458	2468	rVV	98277	167514	5.62%	0.574%
31	17.125	2469	2474	2484	rVB5	29398	71219	2.39%	0.244%
32	17.219	2486	2490	2496	rVB2	19322	37608	1.26%	0.129%
33	17.302	2499	2504	2510	rBV7	16150	38184	1.28%	0.131%
34	17.360	2510	2514	2519	rBV	41484	62872	2.11%	0.216%
35	17.466	2529	2532	2538	rVB4	34747	53413	1.79%	0.183%
36	17.754	2573	2581	2585	rBV2	145031	331802	11.13%	1.138%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

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_E\Methods\8270-BE110624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.801	2585	2589	2595	rVV	158249	237942	7.98%	0.816%
38	17.877	2599	2602	2606	rVV	39669	60997	2.05%	0.209%
39	17.948	2610	2614	2618	rVV2	98687	220618	7.40%	0.756%
40	17.989	2618	2621	2630	rVB	93281	138351	4.64%	0.474%
41	18.148	2645	2648	2652	rVB2	28431	36298	1.22%	0.124%
42	18.253	2661	2666	2672	rBV	79453	130288	4.37%	0.447%
43	18.324	2675	2678	2682	rVB	77464	97614	3.27%	0.335%
44	18.541	2711	2715	2718	rBV2	61533	74594	2.50%	0.256%
45	18.582	2719	2722	2729	rVB2	38708	49730	1.67%	0.171%
46	18.665	2732	2736	2741	rBV	109332	168200	5.64%	0.577%
47	18.759	2750	2752	2756	rVB2	52625	62698	2.10%	0.215%
48	18.800	2757	2759	2762	rBV2	24933	33305	1.12%	0.114%
49	18.847	2764	2767	2768	rBV	42307	46096	1.55%	0.158%
50	18.953	2777	2785	2789	rBV	933147	1336722	44.83%	4.583%
51	18.988	2789	2791	2795	rVB2	51008	62261	2.09%	0.213%
52	19.199	2824	2827	2835	rBV3	38167	75986	2.55%	0.261%
53	19.282	2837	2841	2843	rVV2	109097	163016	5.47%	0.559%
54	19.323	2843	2848	2852	rVB	848695	1154398	38.72%	3.958%
55	19.499	2872	2878	2884	rBV	2390960	2981563	100.00%	10.223%
56	19.628	2897	2900	2901	rBV	59664	64114	2.15%	0.220%
57	19.957	2954	2956	2960	rVB	104902	112842	3.78%	0.387%
58	20.104	2977	2981	2984	rBV	110304	143524	4.81%	0.492%
59	20.145	2985	2988	2995	rVB3	145584	209604	7.03%	0.719%
60	20.557	3055	3058	3062	rVB	115634	123165	4.13%	0.422%
61	20.709	3081	3084	3088	rBV3	190214	242065	8.12%	0.830%
62	20.798	3095	3099	3103	rBV2	115267	175248	5.88%	0.601%
63	21.068	3137	3145	3148	rBV2	1469471	2652403	88.96%	9.094%
64	21.103	3148	3151	3156	rVB	682430	852346	28.59%	2.922%
65	22.114	3320	3323	3331	rVB2	208085	314380	10.54%	1.078%
66	22.325	3355	3359	3364	rVB	258549	375857	12.61%	1.289%
67	22.648	3409	3414	3427	rVB	568076	1844903	61.88%	6.325%
68	23.148	3495	3499	3504	rBV	347158	544689	18.27%	1.868%
69	23.248	3511	3516	3523	rBV	380015	676410	22.69%	2.319%
70	23.359	3528	3535	3540	rBV	1084416	2158886	72.41%	7.402%

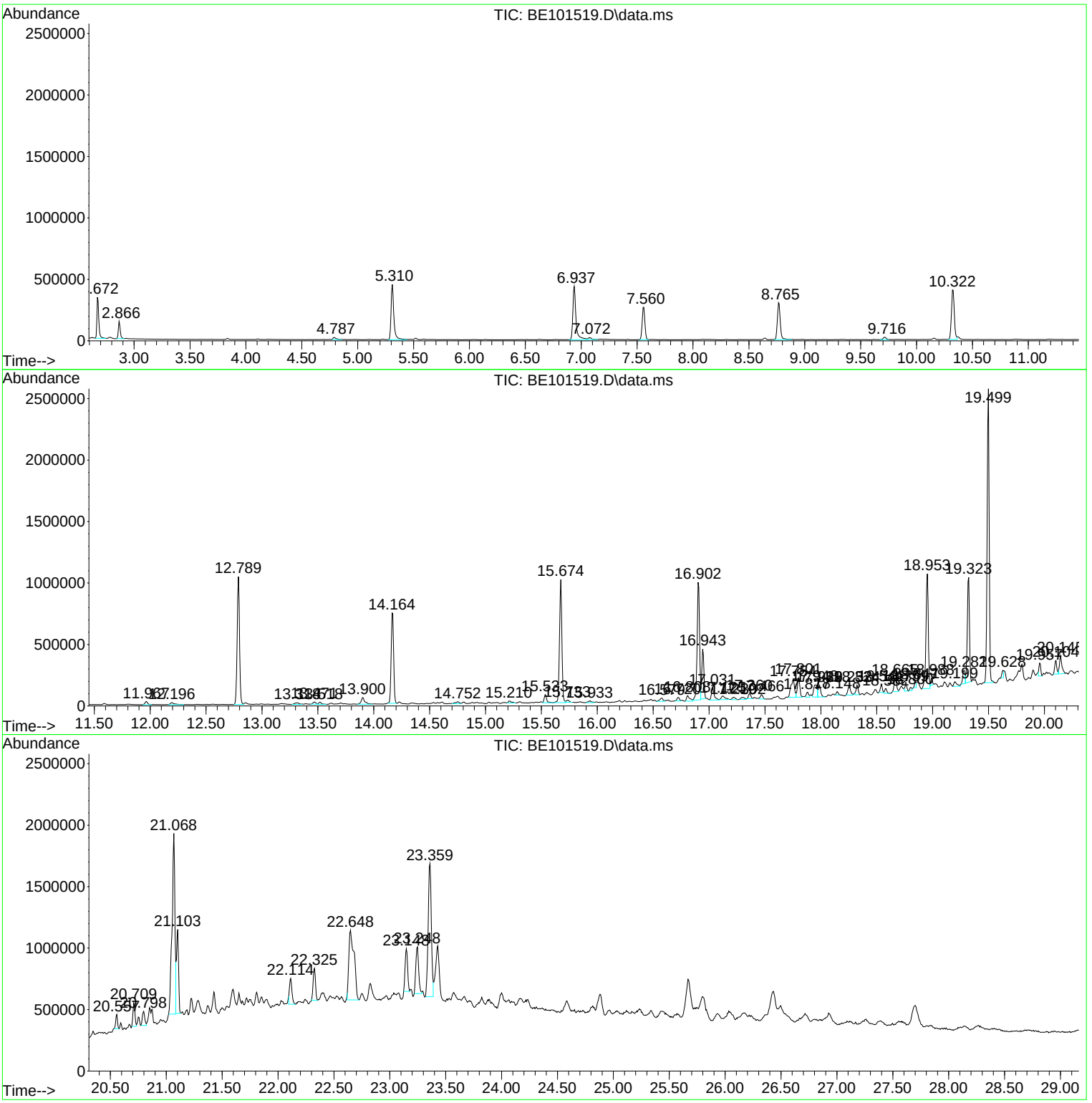
Sum of corrected areas: 29166508

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

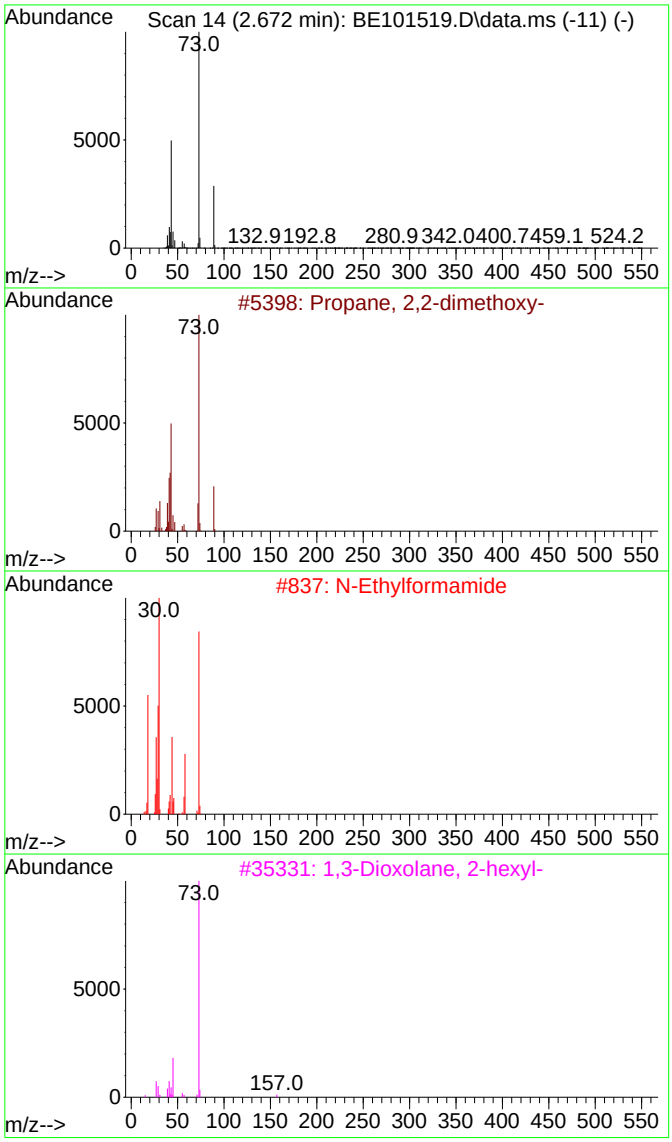
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

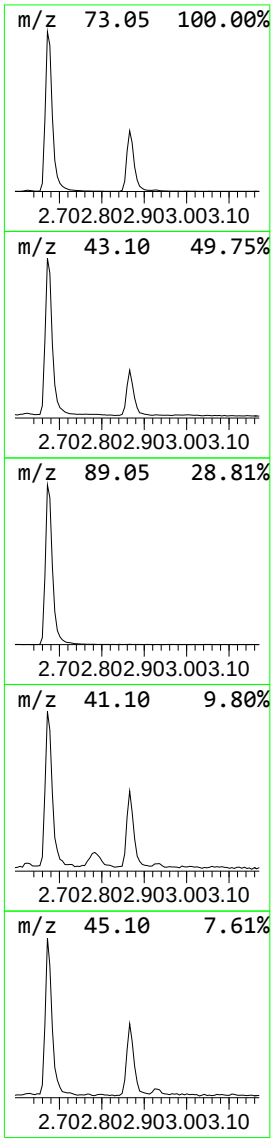
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.672	17.88 ng	388975	1,4-Dichlorobenzene-d4	7.560

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1,3-Dioxolane, 2-hexyl-	158	C9H18O2	001708-34-5	9
4	2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

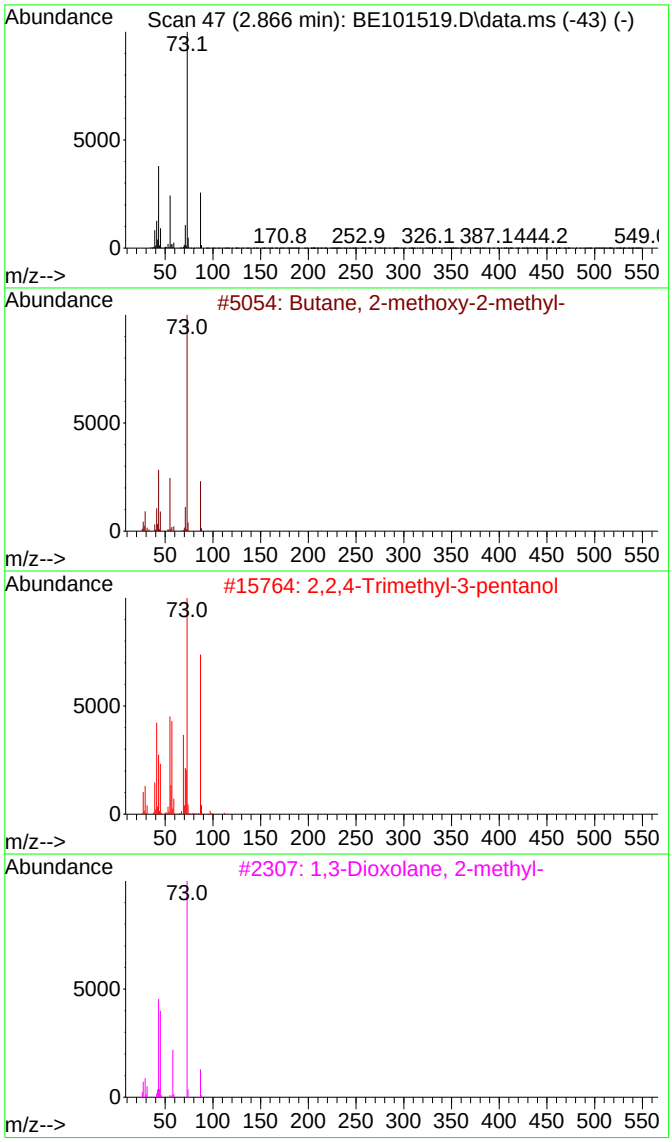
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

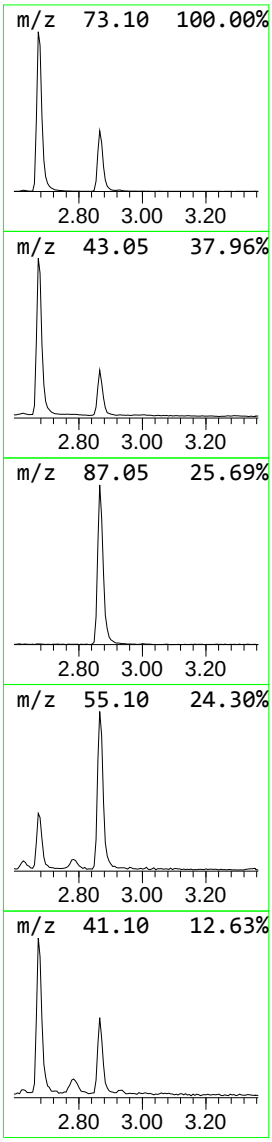
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.866	7.64 ng	166127	1,4-Dichlorobenzene-d4	7.560

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	14
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

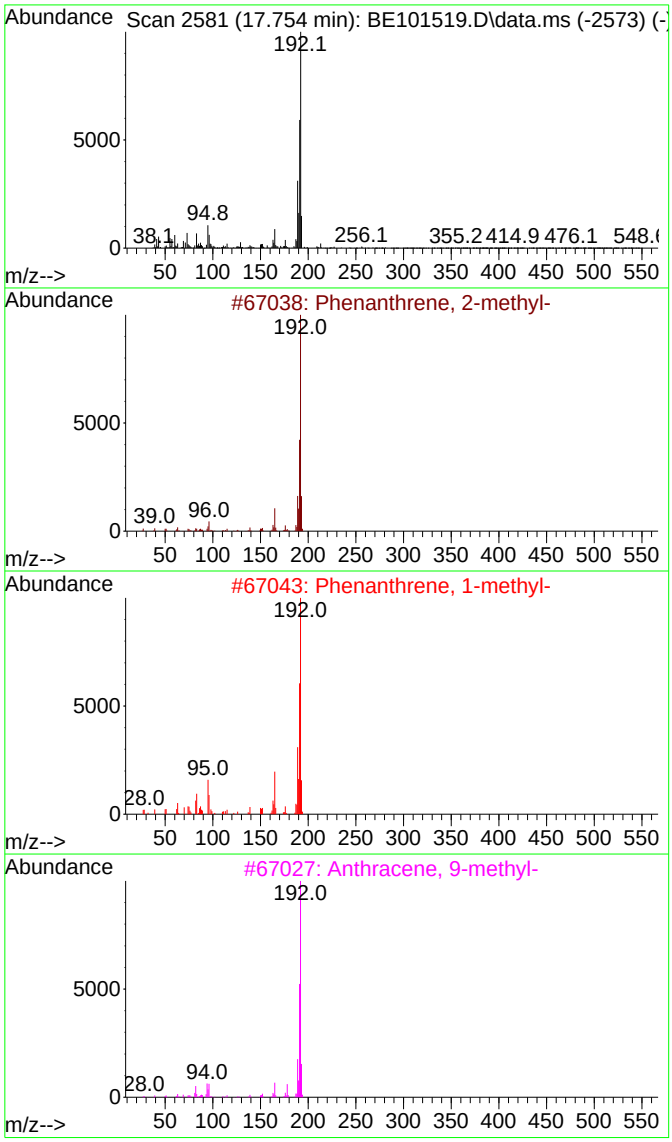
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

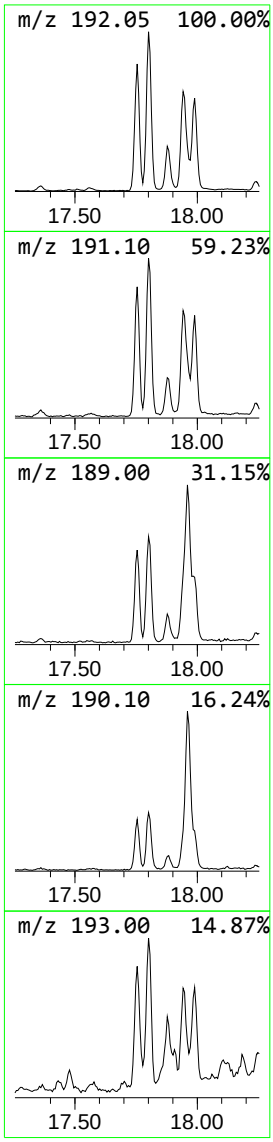
****

Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.754	4.57 ng	331802	Phenanthrene-d10	16.902

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
4	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	93
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

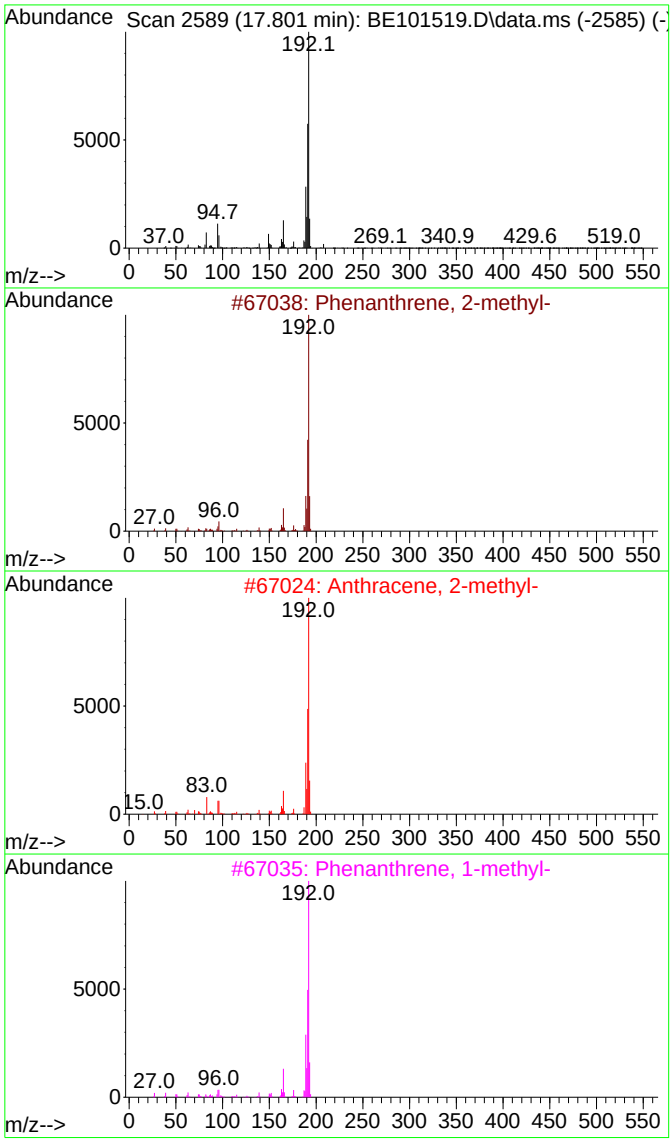
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

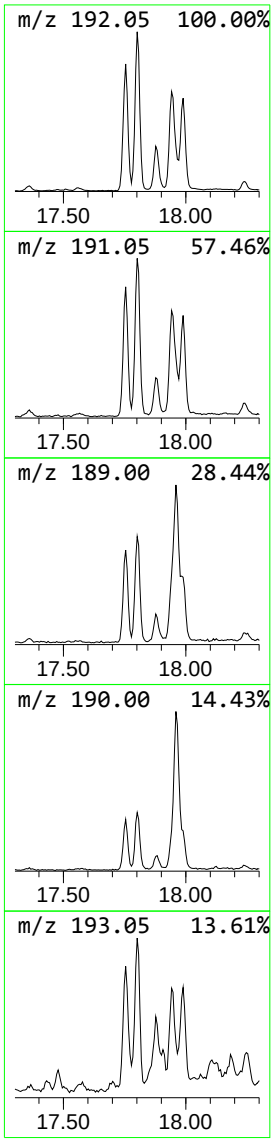
****

Peak Number 4 Anthracene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.801	3.28 ng	237942	Phenanthrene-d10	16.902

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

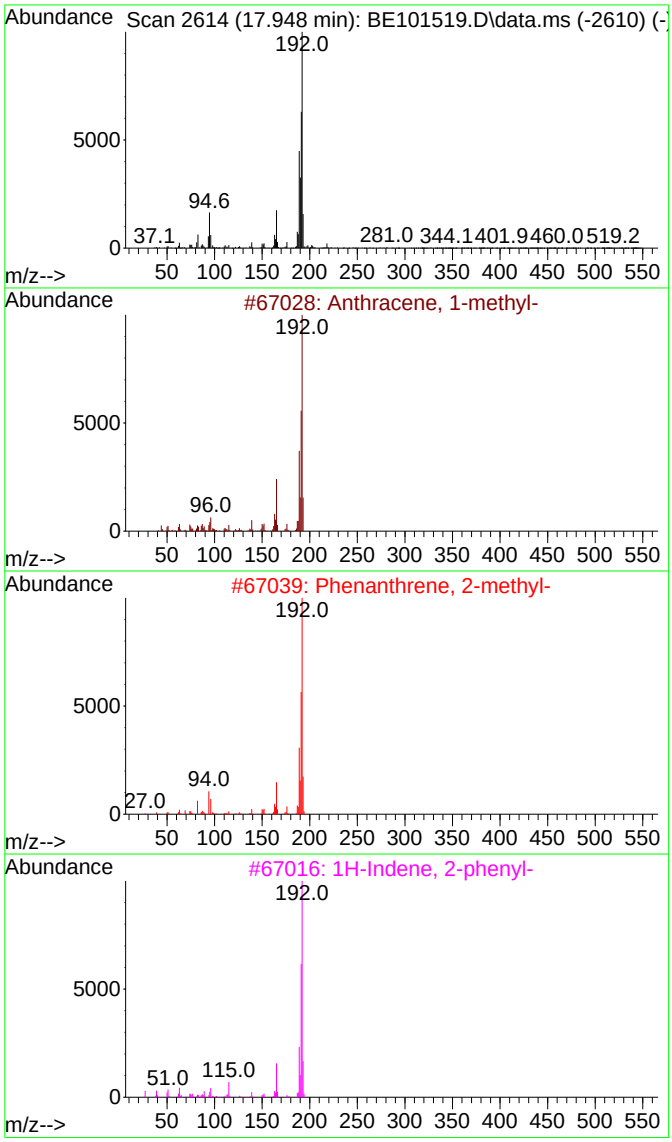
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

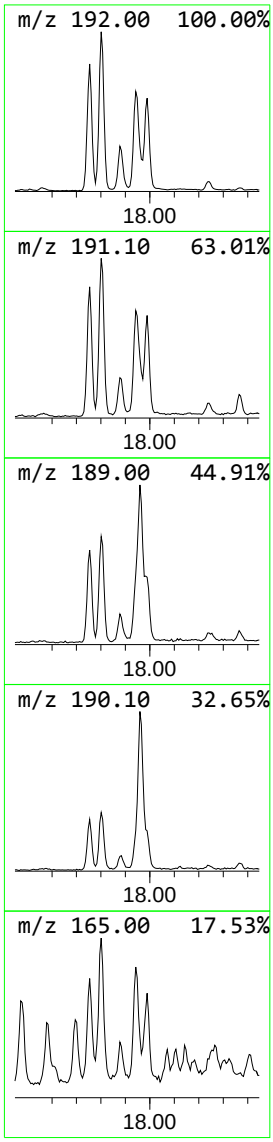
****

Peak Number 5 Anthracene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.948	3.04 ng	220618	Phenanthrene-d10	16.902

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	83
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	76
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	70
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	70
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

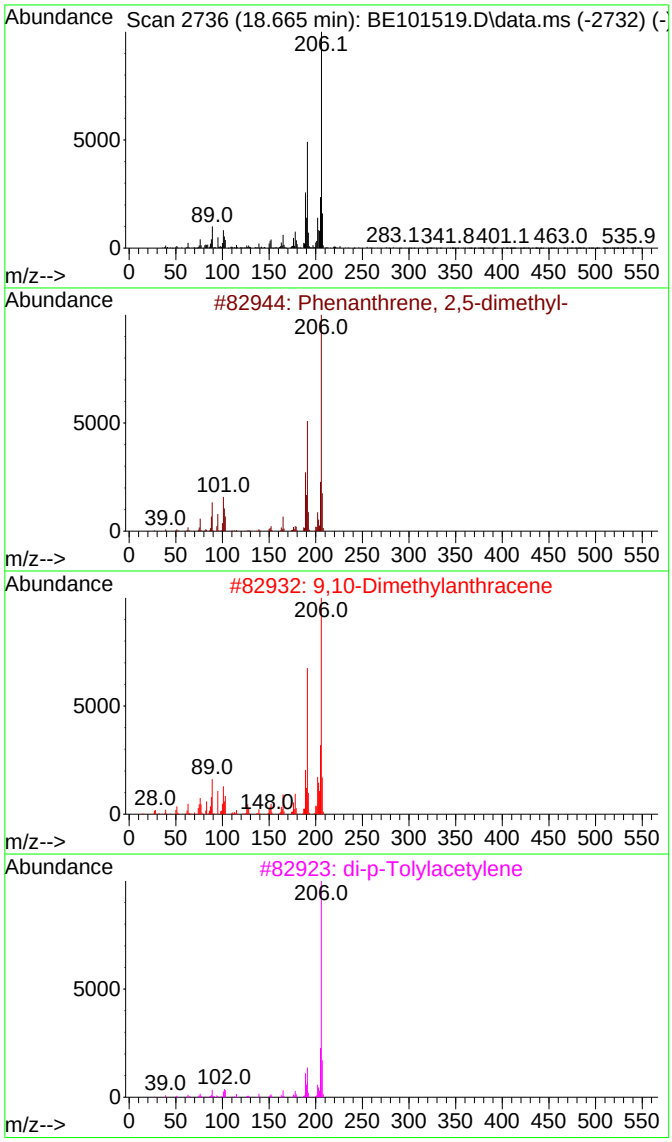
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

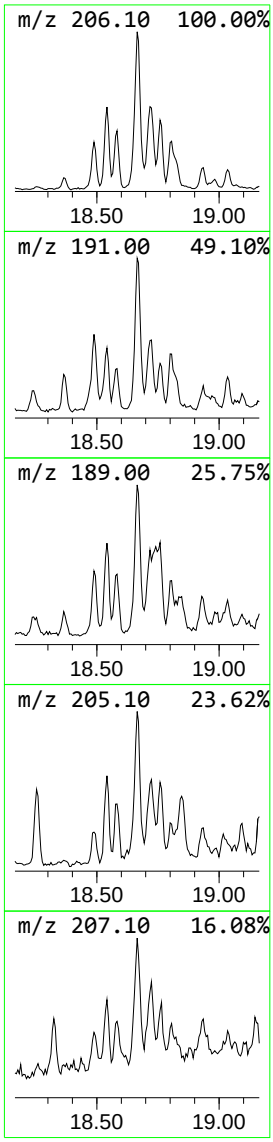
****

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.665	2.32 ng	168200	Phenanthrene-d10	16.902

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	98
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	96
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	93
4	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	93
5	1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

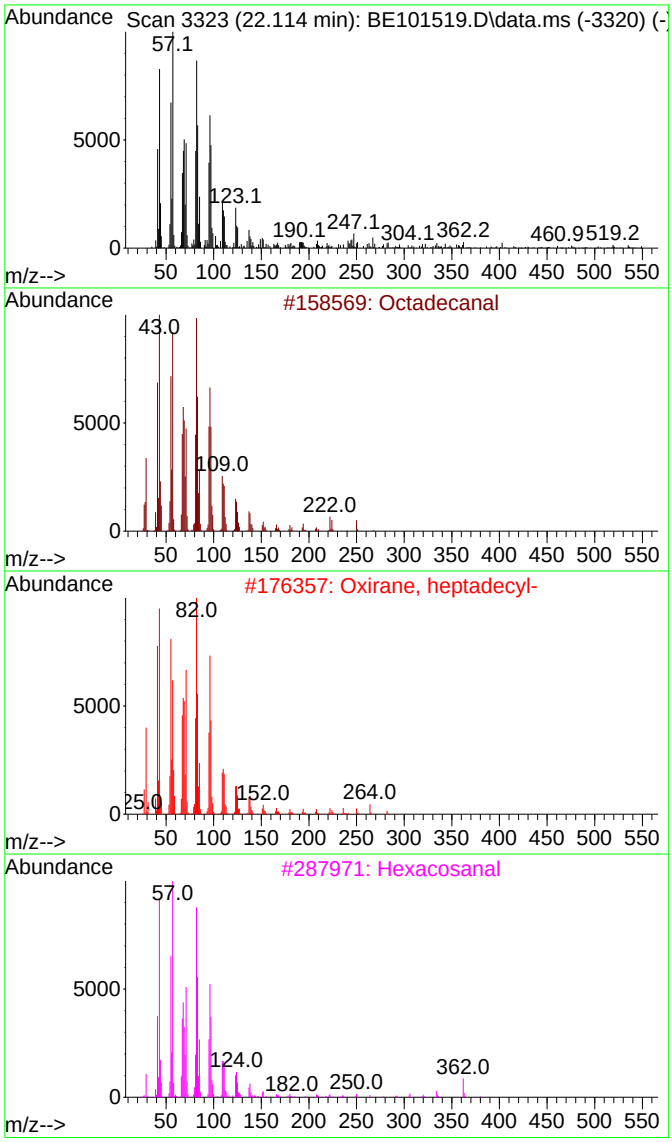
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

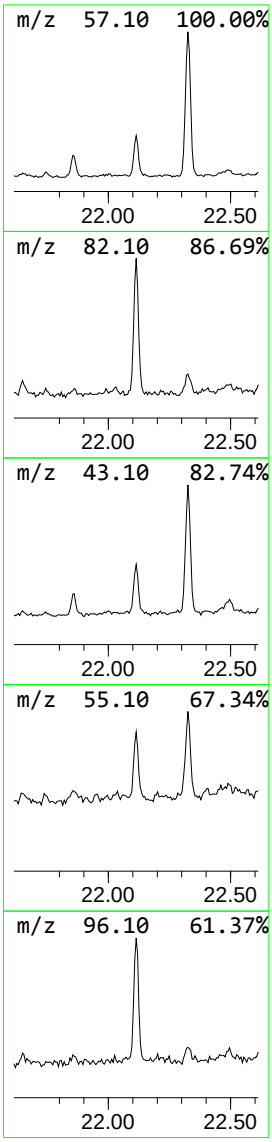
****

Peak Number 7 Octadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.114	2.37 ng	314380	Chrysene-d12	21.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	97
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
3	Hexacosanal	380	C26H52O	026627-85-0	94
4	Tetradecanal	212	C14H28O	000124-25-4	91
5	Pentacosanal	366	C25H50O	058196-28-4	90





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Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CF-613-COMP-16

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

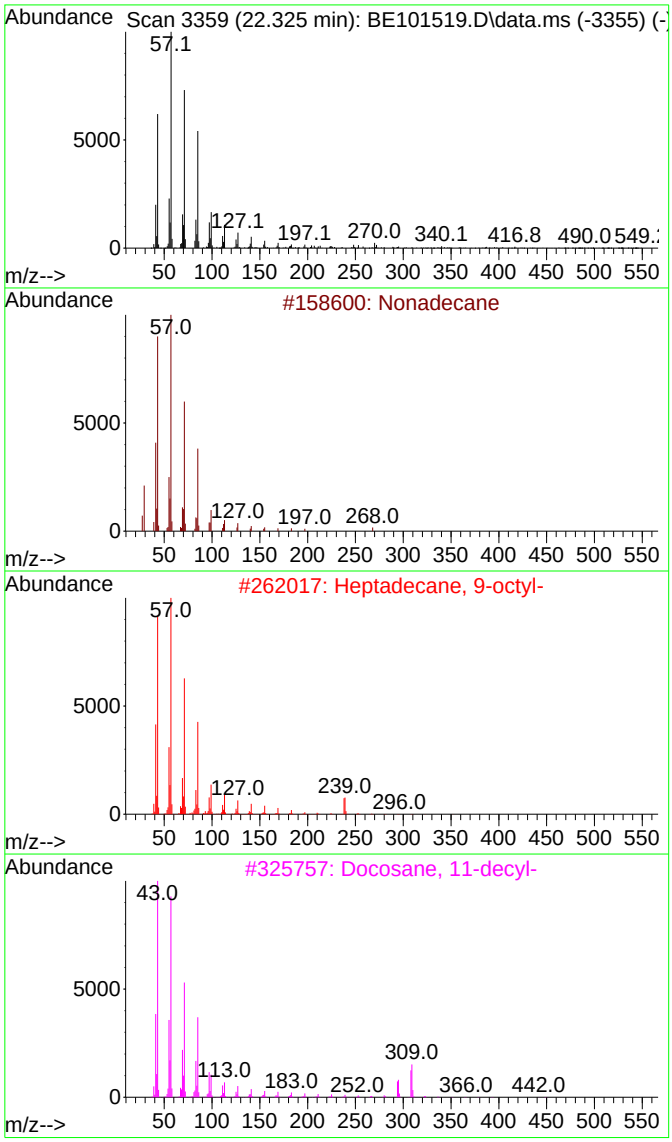
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

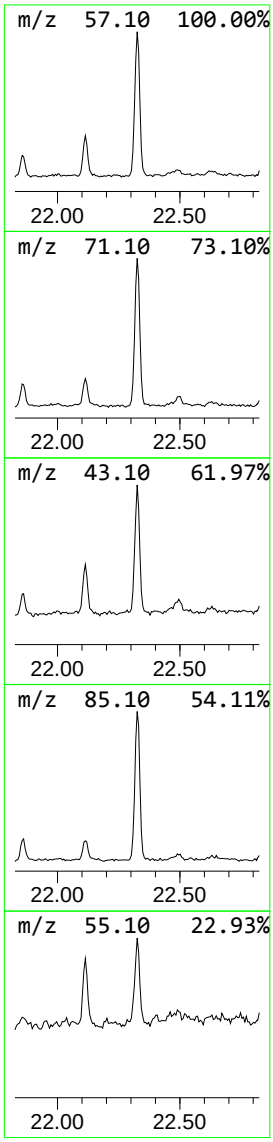
****

Peak Number 8 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.325	3.48 ng	375857	Perylene-d12	23.359

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Docosane, 11-decyl-	451	C32H66	055401-55-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

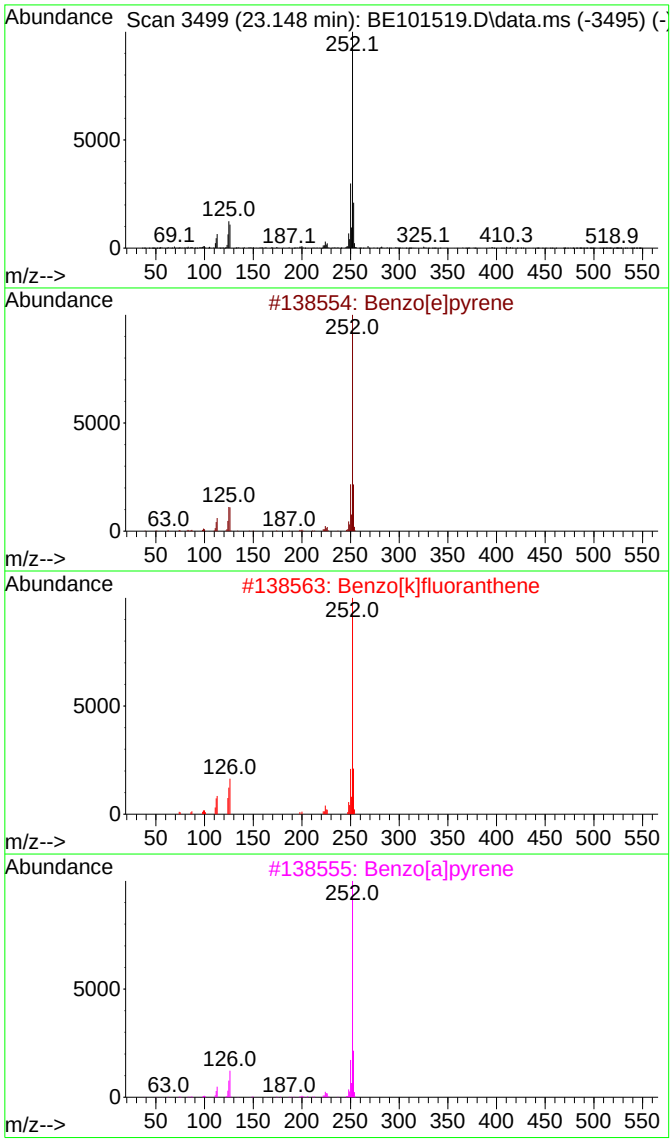
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

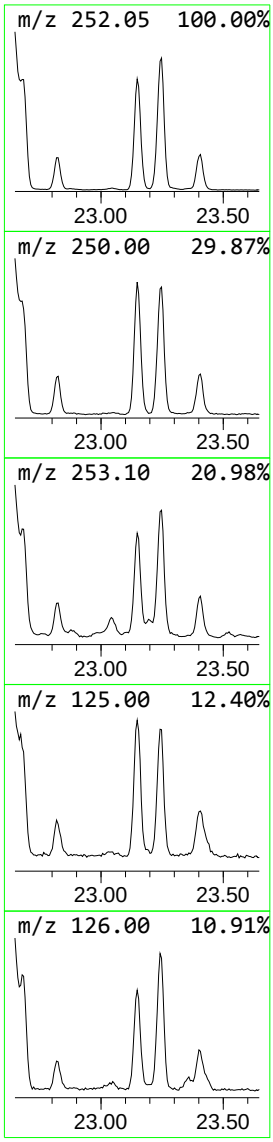
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.148	5.05 ng	544689	Perylene-d12	23.359

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE110624\
Data File : BE101519.D
Acq On : 7 Nov 2024 5:25
Operator : RC/JU
Sample : P4711-01 2X
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
CF-613-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-di...	2.672	17.9	ng	388975	1	7.560	434994	20.0
Butane, 2-metho...	2.866	7.6	ng	166127	1	7.560	434994	20.0
Phenanthrene, 2...	17.754	4.6	ng	331802	4	16.902	1450630	20.0
Anthracene, 2-m...	17.801	3.3	ng	237942	4	16.902	1450630	20.0
Anthracene, 1-m...	17.948	3.0	ng	220618	4	16.902	1450630	20.0
Phenanthrene, 2...	18.665	2.3	ng	168200	4	16.902	1450630	20.0
Octadecanal	22.114	2.4	ng	314380	5	21.068	2652400	20.0
Nonadecane	22.325	3.5	ng	375857	6	23.359	2158890	20.0
Benzo[e]pyrene	23.148	5.0	ng	544689	6	23.359	2158890	20.0